Supplementary Materials

Regulation of RXR-RAR heterodimers by RXR- and RAR- specific ligands and their combinations

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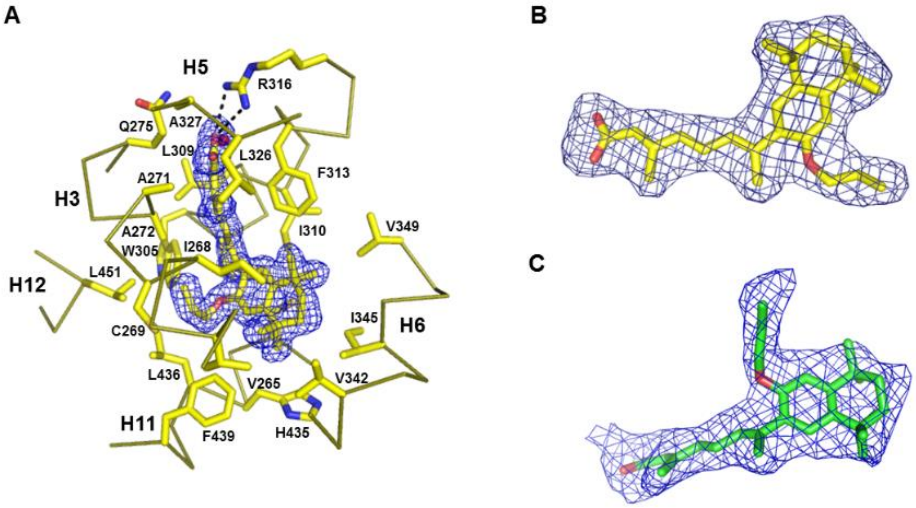
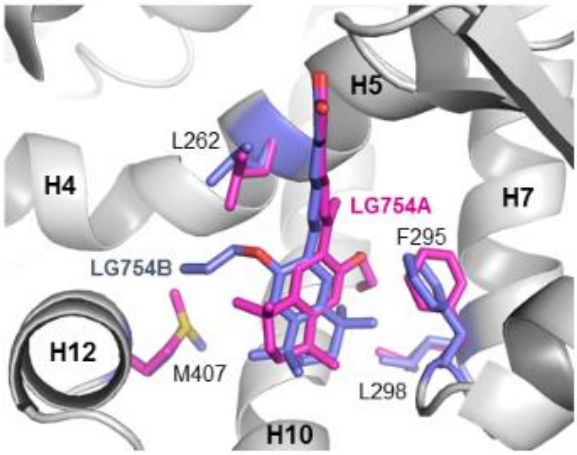
Supplementary Table 1. Data collection and refinement statistics.

Complexe	**RXRα/LG754/TIF2**	**RARβ/LG754/SRC1**
PDB ID	**6STI**	**6SSQ**
Resolution range	46.6 - 1.9 (1.96 - 1.9)	67.2 - 2.3 (2.38 - 2.3)
Space group	P 43 21 2	P 21 21 21
Unit cell	65.96 65.96 111.13	58.21 85.30 109.29
	90 90 90	90 90 90
Total reflections	200743 (18915)	286909 (28587)
Unique reflections	20270 (1975)	24860 (2449)
Multiplicity	9.9 (9.6)	11.5 (11.7)
Completeness (%)	99.95 (99.95)	99.94 (99.84)
Mean I/sigma(I)	51.1 (7.9)	46.5 (3.3)
Wilson B-factor	18.30	31.21
R-merge	0.571 (0.814)	0.759 (2.08)
R-meas	0.602 (0.860)	0.795 (2.18)
R-pim	0.188 (0.272)	0.231 (0.631)
CC1/2	0.72 (0.74)	0.71 (0.44)
CC*	0.92 (0.92)	0.91 (0.78)
Reflections used in refinement	20263 (1974)	24844 (2446)
Reflections used for R-free	1012 (111)	1234 (131)
R-work	0.156 (0.181)	0.164 (0.216)
R-free	0.172 (0.225)	0.209 (0.268)
CC(work)	0.83 (0.86)	0.89 (0.65)
CC(free)	0.79 (0.86)	0.90 (0.63)
Number of non-hydrogen atoms	2103	4215
macromolecules	1783	4012
ligands	33	77
solvent	287	126
Protein residues	225	509
RMS(bonds)	0.011	0.008
RMS(angles)	1.27	1.21
Ramachandran favored (%)	97.3	97.2
Ramachandran allowed (%)	2.7	2.6
Ramachandran outliers (%)	0.00	0.20
Rotamer outliers (%)	0.5	0.00
Clashscore	6.55	4.86
Average B-factor	22.0	44.0
macromolecules	20.4	44.0
ligands	16.3	50.3
solvent	32.1	40.8

Statistics for the highest-resolution shell are shown in parentheses.



Supplementary Figure 1: A. LG754 is shown in its 2Fo-Fc electron density map contoured at 2 σ. Side chains of RXRα LBP residues in interaction with LG754 are shown as yellow sticks. **B. and C.** LG754 modelled into the difference density of each RAR molecules of the asymmetric unit of the RARβ crystal structures. The omit Polder map contoured at 3 σ are shown.



Supplementary Figure 2: Close-up view of the superposition of LG754 in the RARβ LBP from the two complexes present in the asymmetric unit. Side chains of the amino acids that have different positions in both complexes are shown in sticks representation. The main differences observed concern M407 and F295 that are closed to the propoxy group of LG754.