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## **Electronic Supplementary Information**

Interaction energies between two antiandrogenic and one androgenic agonist receptor in the presence of a T877A mutation in prostate cancer: a quantum chemistry analysis

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TABLE S1. CPA interaction in complex with the AR receptor, regions and groups where there is drug-residue interaction, radius and energetic value (in kcal/mol).

Residue         Atomic Group         r (Å)         Energy (ε=10)         Energy (ε=20)         Energy (ε=40)           LEU704         II(C12)H         2         -7.4         -6.3         -6.3           ASN705         III(C12)H         2         -0.4         -0.4         -0.4           LEU707         II(C2)H         2         -2.1         -2.0         -1.9           MET780         III(C15)H         2         -0.7         -0.6         -0.6           ALA877         III(C21)H         2         0.9         0.8         0.8           GLY708         II(C1)H         2.5         -2.1         -2.1         -2.0           GLY711         II(C19)H         2.5         -3.7         -3.6         -3.6           MET742         III(C15)H         2.5         -3.7         -3.6         -3.6           MET745         III(C19)H         2.5         -3.7         -3.6         -3.6           PHE764         II(C22)H; III(C15)H         2.5         -5.0         -4.9         -4.8           LEU873         III(C21)H         2.5         -5.0         -4.9         -4.8           LEU880         III(C21)H         2.5         -2.4         -2.4         <	Complex AR-CPA						
ASN705 II(C12)H 2 -0.4 -0.4 -0.4   LEU707 I(C2)H 2 -2.1 -2.0 -1.9   MET780 III(C15)H 2 -0.7 -0.6 -0.6   ALA877 III(C21)H 2 -0.7 -0.6 -0.6   ALA877 III(C21)H 2 -0.9 -0.8   GLY708 I(C1)H 2.5 -2.1 -2.1 -2.0   GLN711 II(C12)H 2.5 -2.1 -2.1 -2.0   GLN711 II(C12)H 2.5 -3.7 -3.6 -3.6   MET742 III(C15)H 2.5 -3.7 -3.6 -3.6   MET742 III(C15)H 2.5 -3.7 -3.6 -3.6   MET745 II(C19)H 2.5 -3.8 -3.7 -3.7   MET745 II(C19)H 2.5 -5.0 -4.9 -4.8   LEU873 II(C22)H 2.5 -5.0 -4.9 -4.8   LEU873 III(C21)H 2.5 -2.4 -2.3 -2.3   PHE891 III(C21)H 2.5 -2.4 -2.3 -2.3   PHE891 III(C21)H 2.5 -1.2 -1.2 -1.2   MET895 II(C18)H 2.5 -2.6 -2.4 -2.4   PHE697 III(C24)H 3 -0.9 -0.9 -0.9   LEU701 III(C20)O 3 -1.3 -1.3 -1.3 -1.2   MET749 I(C4)H 3 -2.7 -2.6 -2.6   ARG752 I(C3)O3 3 -2.1 -1.4 -1.1   SER778 III(C24)H 3 -2.7 -2.6 -2.6   ARG752 I(C3)O3 3 -2.1 -1.4 -1.1   SER778 III(C24)H 3 -3.2 -2.6 -2.6   VAL746 II(C6)CL 3.5 -1.4 -1.3 -1.3   ILE999 II(C18)H 3.5 -1.0 -1.0 -0.9   LEU768 I(C22)H 4 -0.4 -0.4 -0.4   MET787 III(C24)H 5 -0.3 -0.2 -0.2   PHE878 III(C21)H 5 -0.3 -0.3 -0.2   PHE879 III(C24)H 5 -0.3 -0.2 -0.2   ARG779 III(C24)H 5 -0.3 -0.3 -0.2 -0.2   ALA687 I(C22)H 5 -0.1 -0.1 -0.1   PHE770 III(C24)H 5 -0.3 -0.2 -0.2   ALA687 I(C22)H 5 -5 -0.4 -0.4 -0.4   HIS874 III(C21)H 5.5 -0.6 -0.5 -0.5   GLU709 III(C24)H; I(C1)H 6 -0.3 -0.2 -0.2   ALA748 I(C3)O 6 -0.2 -0.2 -0.2 -0.1   ALA765 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 -0.2   ALA748 I(C3)O 6 -0.7 -0.7 -0.5	Residue	Atomic Group			Energy (ε=20)	Energy (ε=40)	
LEU707   ( C2	LEU704	II(C12)H		-7.4	-6.3	-6.3	
MET780 III(C15)H 2 0.9 0.8 0.8 0.8   GLY708 I(C1)H 2.5 -2.1 -2.1 -2.0   GLN711 II(C12)H 2.5 -3.7 -3.6 -3.6   MET741 II(C9)H 2.5 -3.7 -3.6 -3.6   MET742 III(C15)H 2.5 -3.7 -3.6 -3.6   MET745 II(C19)H 2.5 -3.8 -3.7 -3.6   PHE764 I(C22)H 2.5 -5.0 -4.9 -4.8   LEU873 II(C21)H 2.5 -4.0 -4.0 -3.9   LEU880 III(C21)H 2.5 -2.4 -2.3 -2.3   PHE891 III(C21)H 2.5 -2.4 -2.3 -2.3   PHE895 II(C18)H 2.5 -2.6 -2.4 -2.4   PHE697 III(C24)H 3 -0.9 -0.9 -0.9   LEU701 III(C20)O 3 -1.3 -1.3 -1.2   MET749 I(C4)H 3 -2.7 -2.6 -2.6   ARG752 I(C3)O3 3 -2.1 -1.4 -1.1   SER778 III(C24)H 3 -1.5 -1.5 -1.4   PHE876 III(C24)H 3 -1.5 -1.5 -1.4   PHE876 III(C24)H 3 -3.2 -2.6 -2.6   VAL746 II(C6)CL 3.5 -1.4 -1.3 -1.3   ILE899 II(C18)H 3.5 -1.0 -1.0 -0.9   LEU768 II(C24)H 4 -0.4 -0.4 -0.4   MET789 II(C24)H 5 -0.3 -0.3 -0.2   PHE879 III(C24)H 5 -0.3 -0.3 -0.2   LEU768 II(C22)H 4 -0.4 -0.4 -0.4   MET7879 III(C24)H 5 -0.3 -0.3 -0.2   PHE878 III(C24)H 5 -0.3 -0.2 -0.2   LEU881 III(C21)H 5 -0.3 -0.2 -0.2   LEU881 III(C21)H 5 -0.3 -0.2 -0.2   ALA687 III(C24)H 5.5 -0.6 -0.5 -0.5   GLU709 II(C24)H 5.5 -0.6 -0.5 -0.5   GLU709 II(C34)H 5.5 -0.6 -0.5 -0.5   GLU709 II(C34)H 5.5 -0.6 -0.5 -0.5   GLU706 II(C32)H; II(C1)H 6 -0.3 -0.2 -0.2   O.2 -0.2   O.2 -0.2   O.2 -0.2   O.3 -0.2 -0.2   O.4 -0.4 -0.4   O.4 -0.4   O.4 -0.4   O.5 -0.5   O.5	ASN705	II(C12)H	2	-0.4	-0.4	-0.4	
ALA877 III(C21)H 2 0.9 0.8 0.8 GLY708 I(C1)H 2.5 -2.1 -2.1 -2.0 GLN711 II(C12)H 2.5 -1.3 1.1 1.1 TRP741 II(C9)H 2.5 -3.7 -3.6 -3.6 MET742 III(C15)H 2.5 -3.7 -3.6 -3.6 MET745 II(C19)H 2.5 -3.7 -3.7 -3.7 MET745 II(C19)H 2.5 -3.8 -3.7 -3.7 MET745 II(C22)H 2.5 -5.0 -4.9 -4.8 LEU873 II(C22)H; III(C15)H 2.5 -5.0 -4.9 -4.8 LEU873 III(C21)H 2.5 -4.0 -4.0 -3.9 LEU880 III(C21)H 2.5 -1.2 -1.2 -1.2 MET895 III(C18)H 2.5 -1.2 -1.2 -1.2 MET895 III(C18)H 2.5 -2.6 -2.4 -2.4 PHE697 III(C24)H 3 -0.9 -0.9 -0.9 LEU701 III(C20)O 3 -1.3 -1.3 -1.3 -1.2 MET749 I(C4)H 3 -2.7 -2.6 -2.6 ARG752 I(C3)O3 3 -2.1 -1.4 -1.1 SER778 III(C24)H 3 -1.5 -1.5 -1.5 -1.4 PHE876 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C24)H 3 -1.5 -1.5 -1.5 -1.4 PHE876 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C24)H 3 -1.1 -1.0 -1.0 LEU768 I(C22)H 4 -0.4 -0.4 -0.4 MET787 III(C6)CL 4 -1.1 -1.0 -1.0 ARG779 III(C24)H 5 -0.4 -0.4 -0.4 SER703 I(C22)H 5 -0.1 -0.1 -0.1 PHE770 III(C24)H 5 -0.3 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 -0.2 LEU881 III(C21)H; III(C31)H 5 -0.3 -0.2 -0.2 LEU881 III(C21)H; III(C31)H 5 5 -0.3 -0.2 -0.2 LEU881 III(C22)H; IS5) -5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C3)O 6 -0.7 -0.7 -0.5	LEU707	I(C2)H	2		-2.0	-1.9	
GLY708	MET780						
GLN711    II(C12)H	ALA877	III(C21)H	2	0.9	8.0	8.0	
TRP741 II(C9)H 2.5 -3.7 -3.6 -3.6 MET742 III(C15)H 2.5 -3.7 -3.7 -3.7 -3.7 MET745 II(C19)H 2.5 -3.8 -3.7 -3.6 PHE764 I(C22)H 2.5 -5.0 -4.9 -4.8 LEU873 II(C22)H; III(C15)H 2.5 -5.0 -4.9 -4.8 LEU873 III(C22)H; III(C15)H 2.5 -2.4 -2.3 -2.3 PHE891 III(C21)H 2.5 -2.4 -2.3 -2.3 PHE891 III(C21)H 2.5 -1.2 -1.2 -1.2 MET895 III(C18)H 2.5 -2.6 -2.6 -2.4 -2.4 PHE697 III(C24)H 3 -0.9 -0.9 -0.9 LEU701 IIII(C20)O 3 -1.3 -1.3 -1.3 -1.2 MET749 I(C4)H 3 -2.7 -2.6 -2.6 ARG752 I(C3)O3 3 -2.1 -1.4 -1.1 SER778 III(C24)H 3 -1.5 -1.5 -1.5 -1.4 PHE876 IIII(C24)H 3 -1.5 -1.5 -1.5 -1.4 PHE876 IIII(C24)H 3 -3.2 -2.6 -2.6 VAL746 III(C6)CL 3.5 -1.4 -1.3 -1.3 ILE899 III(C18)H 3.5 -1.0 -1.0 -0.9 LEU768 I(C22)H 4 -0.4 -0.4 -0.4 MET787 III(C6)CL 4 -1.1 -1.0 -1.0 ARG779 IIII(C24)H 4.5 -0.4 -0.4 -0.4 MET787 III(C6)CL 4 -1.1 -1.0 -1.0 ARG779 IIII(C24)H 5 -0.3 -0.2 -0.2 PHE878 IIII(C24)H 5 -0.3 -0.3 -0.2 PHE878 IIII(C24)H 5 -0.3 -0.3 -0.2 PHE878 IIII(C24)H 5 -0.3 -0.3 -0.2 PHE878 IIII(C24)H 5 -0.3 -0.2 -0.2 LEU881 IIII(C21)H; III(C21)H 5 -0.3 -0.2 -0.2 -0.2 LEU881 IIII(C24)H 5.5 -0.1 -0.1 -0.1 LEU700 IIII(C24)H 5.5 -0.1 -0.1 -0.1 LEU700 IIII(C24)H 5.5 -0.4 -0.4 -0.4 -0.4 -0.4 IIII(C24)H 5.5 -0.3 -0.2 -0.2 -0.2 ALA687 III(C22)H 5.5 -0.6 -0.5 -0.5 GLU709 III(C24)H 5.5 -0.6 -0.2 -0.2 -0.2 -0.2 ALA748 III(C15)H 6 -0.3 -0.2 -0.2 -0.2 -0.2 ALA748 III(C3)O 6 -0.2 -0.2 -0.2 -0.2 -0.1 ALA765 III(C22)H; III(C3)O 6 -0.7 -0.7 -0.5	GLY708		2.5		-2.1	-2.0	
MET742         III(C15)H         2.5         -3.7         -3.7         -3.7           MET745         III(C19)H         2.5         -3.8         -3.7         -3.6           PHE764         I(C22)H;         2.5         -5.0         -4.9         -4.8           LEU873         III(C22)H; III(C15)H         2.5         -5.0         -4.0         -3.9           LEU880         IIII(C21)H         2.5         -2.4         -2.3         -2.3           PHE891         III(C21)H         2.5         -2.6         -2.4         -2.3         -2.3           PHE895         III(C21)H         2.5         -1.2         -1.2         -1.2         -1.2           MET895         III(C24)H         3         -0.9         -0.9         -0.9         -0.9           LEU701         III(C24)H         3         -0.9         -0.9         -0.9           LEU701         III(C20)O         3         -1.3         -1.3         -1.2           MET749         I(C4)H         3         -2.7         -2.6         -2.6           ARG752         I(C3)O3         3         -2.1         -1.4         -1.1           SER778         III(C24)H         3         -1.5 <td></td> <td>II(C12)H</td> <td>2.5</td> <td>1.3</td> <td></td> <td>1.1</td>		II(C12)H	2.5	1.3		1.1	
MET745         II(C19)H         2.5         -3.8         -3.7         -3.6           PHE764         I(C22)H; II(C15)H         2.5         -5.0         -4.9         -4.8           LEU873         II(C22)H; III(C15)H         2.5         -5.0         -4.0         -3.9           LEU880         III(C21)H         2.5         -2.4         -2.3         -2.3           PHE891         III(C21)H         2.5         -1.2         -1.2         -1.2           MET895         III(C24)H         3         -0.9         -0.9         -0.9           LEU701         III(C24)H         3         -0.9         -0.9         -0.9           LEU701         III(C24)H         3         -2.7         -2.6         -2.6           ARG752         I(C3)O3         3         -1.3         -1.3         -1.2           MET749         II(C24)H         3         -1.5         -1.5         -1.4           PHE876         III(C24)H         3         -1.5         -1.5         -1.4           PHE876         III(C24)H         3         -3.2         -2.6         -2.6           VAL746         III(C6)CL         3.5         -1.4         -1.3         -1.3	TRP741	II(C9)H	2.5	-3.7	-3.6	-3.6	
PHE764		III(C15)H	2.5				
LEU873         III(C22)H; III(C15)H         2.5         -4.0         -4.0         -3.9           LEU880         III(C21)H         2.5         -2.4         -2.3         -2.3           PHE891         III(C21)H         2.5         -1.2         -1.2         -1.2         -1.2           MET895         III(C18)H         2.5         -2.6         -2.4         -2.4         -2.4           PHE697         III(C24)H         3         -0.9         -0.9         -0.9         -0.9           LEU701         III(C20)O         3         -1.3         -1.3         -1.2         -0.9           MET749         I(C4)H         3         -2.7         -2.6         -2.6         -2.6           ARG752         I(C3)O3         3         -2.1         -1.4         -1.1         -1.5         -1.4         -1.1           SER778         III(C24)H         3         -3.2         -2.6         -2.6         -2.6           VAL746         III(C6)CL         3.5         -1.4         -1.3         -1.3         -1.3           ILE899         III(C18)H         3.5         -1.0         -1.0         -0.9           LEU768         I(C22)H         4         -0.4							
LEU880 III(C21)H 2.5 -2.4 -2.3 -2.3 PHE891 III(C21)H 2.5 -1.2 -1.2 -1.2 MET895 III(C18)H 2.5 -2.6 -2.4 -2.4 PHE697 III(C24)H 3 -0.9 -0.9 -0.9 LEU701 III(C20)O 3 -1.3 -1.3 -1.2 MET749 I(C4)H 3 -2.7 -2.6 -2.6 ARG752 I(C3)O3 3 -2.1 -1.4 -1.1 SER778 III(C24)H 3 -1.5 -1.5 -1.5 -1.4 PHE876 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 II(C6)CL 3.5 -1.4 -1.3 -1.3 ILE899 III(C18)H 3.5 -1.0 -1.0 -0.9 LEU768 I(C22)H 4 -0.4 -0.4 -0.4 MET787 III(C6)CL 4 -1.1 -1.0 -1.0 ARG779 III(C24)H 4.5 -0.4 -0.4 -0.4 SER703 I(C22)H 4.5 -0.4 -0.4 -0.4 SER703 I(C22)H 5 -0.1 -0.1 -0.1 PHE770 III(C24)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 -0.2 LEU881 III(C21)H 5 -0.2 -0.2 -0.2 ALA687 I(C22)H 5.5 -0.1 -0.1 -0.1 -0.1 LEU700 III(C24)H 5.5 -0.4 -0.4 -0.4 -0.3 GLU709 I(C1)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 -0.2 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O							
PHE891							
MET895         II(C18)H         2.5         -2.6         -2.4         -2.4           PHE697         III(C24)H         3         -0.9         -0.9         -0.9           LEU701         III(C20)O         3         -1.3         -1.3         -1.2           MET749         I(C4)H         3         -2.7         -2.6         -2.6           ARG752         I(C3)O3         3         -2.1         -1.4         -1.1           SER778         IIII(C24)H         3         -1.5         -1.5         -1.4           PHE876         IIII(C24)H         3         -3.2         -2.6         -2.6           VAL746         II(C6)CL         3.5         -1.4         -1.3         -1.3           ILE899         II(C18)H         3.5         -1.0         -1.0         -0.9           LEU768         I(C22)H         4         -0.4         -0.4         -0.4           MET787         III(C6)CL         4         -1.1         -1.0         -1.0           ARG779         IIII(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770 <td></td> <td></td> <td></td> <td></td> <td></td> <td>-2.3</td>						-2.3	
PHE697 III(C24)H 3 -0.9 -0.9 -0.9 LEU701 III(C20)O 3 -1.3 -1.3 -1.2 MET749 I(C4)H 3 -2.7 -2.6 -2.6 ARG752 I(C3)O3 3 -2.1 -1.4 -1.1 SER778 III(C24)H 3 -1.5 -1.5 -1.4 PHE876 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 II(C6)CL 3.5 -1.4 -1.3 -1.3 ILE899 II(C18)H 3.5 -1.0 -1.0 -0.9 LEU768 I(C22)H 4 -0.4 -0.4 -0.4 MET787 II(C6)CL 4 -1.1 -1.0 -1.0 ARG779 III(C24)H 4.5 -0.4 -0.4 -0.4 SER703 I(C22)H 5 -0.1 -0.1 -0.1 PHE770 III(C24)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.2 -0.2 LEU881 III(C21)H 5 -0.2 -0.2 LEU881 III(C21)H 5 -0.2 -0.2 ALA687 I(C22)H 5.5 -0.1 -0.1 -0.1 -0.1 LEU700 III(C24)H 5.5 -0.4 -0.4 -0.4 -0.4 -0.4 III(C30)H 5.5 -0.5 -0.5 GLU709 I(C1)H 5.5 -0.6 -0.5 -0.5 GLU709 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 -0.7 0.7 0.5 -0.5							
LEU701 III(C20)O 3 -1.3 -1.3 -1.2 MET749 I(C4)H 3 -2.7 -2.6 -2.6 ARG752 I(C3)O3 3 -2.1 -1.4 -1.1 SER778 III(C24)H 3 -1.5 -1.5 -1.4 PHE876 III(C24)H 3 -3.2 -2.6 -2.6 VAL746 II(C6)CL 3.5 -1.4 -1.3 -1.3 ILE899 II(C18)H 3.5 -1.0 -1.0 -0.9 LEU768 I(C22)H 4 -0.4 -0.4 -0.4 MET787 II(C6)CL 4 -1.1 -1.0 -1.0 ARG779 III(C24)H 4.5 -0.4 -0.4 -0.4 SER703 I(C22)H 5 -0.1 -0.1 -0.1 PHE770 III(C24)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 -0.2 LEU881 III(C21)H 5 -0.2 -0.2 -0.2 LEU881 III(C21)H 5.5 -0.1 -0.1 -0.1 -0.1 LEU700 III(C24)H 5.5 -0.4 -0.4 -0.4 -0.4 -0.3 GLU709 I(C1)H 5.5 -0.4 -0.4 -0.4 -0.3 GLU709 I(C1)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.2 -0.1	MET895	II(C18)H	2.5	-2.6		-2.4	
MET749         I(C4)H         3         -2.7         -2.6         -2.6           ARG752         I(C3)O3         3         -2.1         -1.4         -1.1           SER778         III(C24)H         3         -1.5         -1.5         -1.4           PHE876         III(C24)H         3         -3.2         -2.6         -2.6           VAL746         II(C6)CL         3.5         -1.4         -1.3         -1.3           ILE899         II(C18)H         3.5         -1.0         -1.0         -0.9           LEU768         I(C22)H         4         -0.4         -0.4         -0.4           MET787         II(C6)CL         4         -1.1         -1.0         -1.0           ARG779         III(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H         5         -0.2         -0.2         -0.2           ALA687	PHE697		3				
ARG752	LEU701	III(C20)O		-1.3			
SER778         III(C24)H         3         -1.5         -1.5         -1.4           PHE876         III(C24)H         3         -3.2         -2.6         -2.6           VAL746         II(C6)CL         3.5         -1.4         -1.3         -1.3           ILE899         II(C18)H         3.5         -1.0         -1.0         -0.9           LEU768         I(C22)H         4         -0.4         -0.4         -0.4           MET787         II(C6)CL         4         -1.1         -1.0         -1.0           ARG779         III(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3	MET749	I(C4)H		-2.7	-2.6	-2.6	
PHE876         III(C24)H         3         -3.2         -2.6         -2.6           VAL746         II(C6)CL         3.5         -1.4         -1.3         -1.3           ILE899         II(C18)H         3.5         -1.0         -1.0         -0.9           LEU768         I(C22)H         4         -0.4         -0.4         -0.4           MET787         II(C6)CL         4         -1.1         -1.0         -1.0           ARG779         III(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.3         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3           GLU709         I(C1)H         5.5         -0.6         -0.5         -0.5           <	ARG752					-1.1	
VAL746	SER778	III(C24)H		-1.5	-1.5	-1.4	
ILE899	PHE876	III(C24)H	3		-2.6	-2.6	
LEU768         I(C22)H         4         -0.4         -0.4         -0.4           MET787         III(C6)CL         4         -1.1         -1.0         -1.0           ARG779         III(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3         -0.2         -0.3           GLU709         I(C1)H         5.5         -1.7         -0.5         -0.4           HIS874         III(C15)H         5.5         -0.6         -0.5         -0.5           GLU706         I(C22)H; I(C1)H         6         -0.3         -0.2         -0.2           ALA748         I(C3)O         6         -0.2	VAL746	II(C6)CL	3.5	-1.4	-1.3	-1.3	
MET787         II(C6)CL         4         -1.1         -1.0         -1.0           ARG779         III(C24)H         4.5         -0.4         -0.4         -0.4           SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3           GLU709         I(C1)H         5.5         -1.7         -0.5         -0.4           HIS874         III(C15)H         5.5         -0.6         -0.5         -0.5           GLU706         I(C22)H; I(C1)H         6         -0.3         -0.2         -0.2           ALA748         I(C3)O         6         -0.2         -0.2         -0.1           ALA765         I(C22)H; I(C3)O         6         0.7         0.7         0.5	ILE899	II(C18)H				-0.9	
ARG779 III(C24)H 4.5 -0.4 -0.4 -0.4 SER703 I(C22)H 5 -0.1 -0.1 -0.1 -0.1 PHE770 III(C24)H 5 -0.3 -0.3 -0.2 PHE878 III(C21)H 5 -0.3 -0.2 -0.2 LEU881 III(C21)H; III(C21)H 5 -0.2 -0.2 -0.2 ALA687 I(C22)H 5.5 -0.1 -0.1 -0.1 LEU700 III(C24)H 5.5 -0.4 -0.4 -0.3 GLU709 I(C1)H 5.5 -1.7 -0.5 -0.4 HIS874 III(C15)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5	LEU768	I(C22)H	4	-0.4	-0.4	-0.4	
SER703         I(C22)H         5         -0.1         -0.1         -0.1           PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3           GLU709         I(C1)H         5.5         -1.7         -0.5         -0.4           HIS874         III(C15)H         5.5         -0.6         -0.5         -0.5           GLU706         I(C22)H; I(C1)H         6         -0.3         -0.2         -0.2           ALA748         I(C3)O         6         -0.2         -0.2         -0.1           ALA765         I(C22)H; I(C3)O         6         0.7         0.7         0.5	MET787	II(C6)CL	4	-1.1	-1.0	-1.0	
PHE770         III(C24)H         5         -0.3         -0.3         -0.2           PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3           GLU709         I(C1)H         5.5         -1.7         -0.5         -0.4           HIS874         III(C15)H         5.5         -0.6         -0.5         -0.5           GLU706         I(C22)H; I(C1)H         6         -0.3         -0.2         -0.2           ALA748         I(C3)O         6         -0.2         -0.2         -0.1           ALA765         I(C22)H; I(C3)O         6         0.7         0.7         0.5			4.5				
PHE878         III(C21)H         5         -0.3         -0.2         -0.2           LEU881         III(C21)H; III(C21)H         5         -0.2         -0.2         -0.2           ALA687         I(C22)H         5.5         -0.1         -0.1         -0.1           LEU700         III(C24)H         5.5         -0.4         -0.4         -0.3           GLU709         I(C1)H         5.5         -1.7         -0.5         -0.4           HIS874         III(C15)H         5.5         -0.6         -0.5         -0.5           GLU706         I(C22)H; I(C1)H         6         -0.3         -0.2         -0.2           ALA748         I(C3)O         6         -0.2         -0.2         -0.1           ALA765         I(C22)H; I(C3)O         6         0.7         0.7         0.5			5				
LEU881       III(C21)H; III(C21)H       5       -0.2       -0.2       -0.2         ALA687       I(C22)H       5.5       -0.1       -0.1       -0.1         LEU700       III(C24)H       5.5       -0.4       -0.4       -0.3         GLU709       I(C1)H       5.5       -1.7       -0.5       -0.4         HIS874       III(C15)H       5.5       -0.6       -0.5       -0.5         GLU706       I(C22)H; I(C1)H       6       -0.3       -0.2       -0.2         ALA748       I(C3)O       6       -0.2       -0.2       -0.1         ALA765       I(C22)H; I(C3)O       6       0.7       0.7       0.5							
ALA687 I(C22)H 5.5 -0.1 -0.1 -0.1 LEU700 III(C24)H 5.5 -0.4 -0.4 -0.3 GLU709 I(C1)H 5.5 -1.7 -0.5 -0.4 HIS874 III(C15)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5	PHE878						
LEU700     III(C24)H     5.5     -0.4     -0.4     -0.3       GLU709     I(C1)H     5.5     -1.7     -0.5     -0.4       HIS874     III(C15)H     5.5     -0.6     -0.5     -0.5       GLU706     I(C22)H; I(C1)H     6     -0.3     -0.2     -0.2       ALA748     I(C3)O     6     -0.2     -0.2     -0.1       ALA765     I(C22)H; I(C3)O     6     0.7     0.7     0.5							
GLU709 I(C1)H 5.5 -1.7 -0.5 -0.4 HIS874 III(C15)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5							
HIS874 III(C15)H 5.5 -0.6 -0.5 -0.5 GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5							
GLU706 I(C22)H; I(C1)H 6 -0.3 -0.2 -0.2 ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5							
ALA748 I(C3)O 6 -0.2 -0.2 -0.1 ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5							
ALA765 I(C22)H; I(C3)O 6 0.7 0.7 0.5							
GL N783 III(C15)H 6 -0.2 -0.2 -0.2							
	GLN783	III(C15)H		-0.2	-0.2	-0.2	
ARG710 I(C1)H; I(C2)H 6.5 -0.2 -0.2 -0.2							
LEU712 I(C1)H; I(C2)H 6.5 -0.1 -0.1 -0.1							
PHE747 II(C6)CL 6.5 -0.1 -0.1 -0.1							
GLY750 I(C4)H 6.5 0.0 0.0 0.0							
LEU762 II(C6)CL 6.5 -0.2 -0.2 -0.2							
TYR763 I(C3)O 6.5 -0.1 -0.1 -0.1							
LYS777 III(C24)H 6.5 0.1 0.0 0.0							
CYS784 III(C24)H 6.5 -0.2 -0.2 0.0							
ILE869 II(C6)CL; II(C22)H 6.5 -0.2 -0.2 -0.1							
ALA870 II(C22)H 6.5 -0.2 -0.2 -0.1							
GLU872 III(C16)H; III(C15)H 6.5 -0.2 -0.2 -0.1		, , , , , , , , , , , , , , , , , , , ,					
GLN875 III(C16)H 6.5 -0.2 -0.2 -0.2							
ASP879 III(C21)H 6.5 -0.3 -0.2 -0.2							
SER884 III(C21)H; III(C21)H 6.5 -0.1 0.0 0.0							
PRO892 II(C18)H; II(C12)H 6.5 -0.1 -0.1 0.0	PRO892	II(C18)H; II(C12)H	6.5	-0.1	-0.1	0.0	

VAL685	I(C2)H	7	-0.1	0.0	0.0
SER702	III(C20)O; III(C24)H	7	-0.1	-0.1	-0.1
VAL715	Ì II(C19)H	7	-0.1	-0.1	-0.1
GLY743	II(C6)CL; II(C19)H	7	-0.1	-0.1	-0.1
LEU744	I(C4)H; II(C19)H	7	-0.1	-0.1	-0.1
MET775	ÍII(C24)H	7	-0.4	-0.1	-0.1
LYS883	III(C21)H	7	-0.8	-0.1	0.0
VAL903	III(C21)H; II(C18)H	7	0.0	0.0	0.0
ARG774	III(C24)H; III(C24)H	7.5	-0.3	-0.1	-0.1
TYR781	III(C24)H; III(C24)H	7.5	-0.2	-0.1	-0.1
ILE882	III(C21)H; III(C21)H	7.5	0.0	0.0	0.0
ALA896	III(C21)H	7.5	-0.1	-0.1	-0.1
CYS686	II(C12)H	8	0.0	0.0	0.0
SER696	III(C24)H	8	0.0	0.0	0.0
ALA698	III(C24)H	8	0.0	0.0	0.0
ALA699	III(C24)H	8	0.0	0.0	0.0
HIS776	III(C24)H	8	0.0	0.0	0.0
LEU790	II(C6)CL	8	0.0	0.0	0.0
ASP890	III(C20)O	8	0.0	0.0	0.0
ILE898	II(C18)H; II(C18)H	8	-0.1	-0.1	0.0
HIS689	I(C22)H	8.5	0.0	0.0	0.0
HIS714	I(C2)H	8.5	0.0	0.0	0.0
SER740	II(C19)H	8.5	0.0	0.0	0.0
SER753	I(C4)H	8.5	0.0	0.0	0.0
VAL866	II(C6)CL	8.5	-0.1	0.0	0.0
ARG871	III(C15)H; III(C15)H	8.5	0.1	0.0	0.0
TRP751	I(C3)O; I(C4)H	9	-0.1	-0.1	0.0
PRO766	I(C2)H; I(C3)O	9	0.0	0.0	0.0
ASP767	I(C22)H	9	0.1	0.0	0.0
VAL769	I(C22)H	9	0.0	0.0	0.0
LEU907	III(C16)H; III(C21)H	9	0.0	0.0	0.0
GLY688	I(C22)H	9.5	0.0	0.0	0.0
VAL713	II(C19)H; II(C19)H	9.5	0.0	0.0	0.0
SER782	III(C24)H	9.5	0.0	0.0	0.0
ARG786	II(C6)CL	9.5	0.0	0.0	0.0
ARG788	II(C6)CL	9.5	0.0	0.0	0.0
HIS885	III(C21)H	9.5	0.0	0.0	0.0
MET894	I(C1)H; II(C11)H	9.5	0.0	0.0	0.0
SER900	III(C21)H	9.5	0.0	0.0	0.0
VAL684	I(C3)O	10	-0.1	0.0	0.0
GLN738	II(C19)H; II(C19)H	10	0.0	0.0	0.0
SER791	I(C4)H; II(C6)CL	10	0.0	0.0	0.0
LYS808	I(C3)O; I(C4)H	10	-0.2	-0.1	-0.1
SER888	III(C21)H	10	0.0	0.0	0.0
VAL889	III(C21)H	10	0.0	0.0	0.0
PRO682	I(C3)O	10.5	0.0	0.0	0.0
ILE737	II(C19)H	10.5	0.0	0.0	0.0
TYR739	II(C19)H	10.5	-0.1	-0.1	-0.1
ASN756	I(C3)O	10.5	-0.1	0.0	0.0
TYR773	III(C24)H	10.5	0.0	0.0	0.0
VAL785	II(C6)CL; III(C24)H	10.5	0.0	0.0	0.0
PHE794	II(C6)CL; I(C4)H	10.5	0.0	0.0	0.0
PHE804	II(C6)CL, I(C4)H I(C3)O	10.5	0.0	0.0	0.0
LEU811	I(C4)H	10.5	0.0	0.0	
PRO868					0.0
PhU008	II(C22)H; III(C15)H	10.5	0.0	0.0	0.0

GLU897	III(C21)H	10.5	-0.1	-0.1	0.0
PRO904	III(C21)H	10.5	0.0	0.0	0.0
GLY683	I(C2)H; I(C3)O	11	0.1	0.0	0.0
ASP695	III(C24)H; III(C24)H	11	0.0	0.0	0.0
VAL716	II(C19)H	11	0.0	0.0	0.0
MET761	I(C4)H	11	0.0	0.0	0.0
GLN867	II(C22)H	11	-0.1	-0.1	0.0
GLU893	II(C11)H; II(C18)H	11	-0.1	-0.1	0.0

TABLE S2. HFT interaction in complex with the AR receptor, regions and groups where there is drug-residue interaction, radius and energetic value (in kcal/mol).

Residue	Complex AR-HFT						
ASN705 III(C11)O 2.5 2.8 3.0 3.2 LEU707 II(C5)H 2.5 -1.7 -1.6 -1.6 GLN711 II(C5)H 2.5 -0.5 -0.5 -0.5 -0.5 O.5 MET745 II(C4)N; (IN1)O 2.5 -0.8 -0.8 -0.8 O.8 PHE764 II(C7)F; I(C4)N 2.5 -4.0 -2.7 -2.7 MET895 III(C12)H 2.5 0.8 0.9 0.9 0.9 LEU701 IIII(C13)H 3 -1.9 -1.8 -1.7 GLY708 IIII(C13)H 3 -1.9 -1.8 -1.7 GLY708 IIII(C13)H 3 -1.9 -1.8 -1.7 O.5 O.5 AAGOS2 III(C12)H 3 -1.7 -1.7 -1.7 -1.6 O.5 AAGOS2 III(C12)H 3 -1.7 -1.7 -1.7 -1.6 AAGOS2 III(C12)H 3 -1.7 -1.7 -1.7 -1.6 AAGOS2 III(C12)H 3 -1.7 -1.7 -1.7 -1.6 AAGOS2 III(C12)H 3 -1.7 -1.7 -1.7 -1.7 PHE876 IIII(C13)H 3 -1.9 -1.8 -1.8 O.9 O.9 O.9 AAGOS2 IIII(C13)H 3 -1.7 -1.7 -1.7 -1.6 O.9 AAGOS2 IIII(C12)H 3 -1.7 -1.7 -1.7 -1.6 O.9 AAGOS2 IIII(C12)H 3 -1.7 -1.7 -1.7 O.9 O.9 ALA877 IIII(C12)H 3 -1.5 -1.5 -1.5 -1.4 ILE899 IIII(C12)H 3 -1.5 -1.5 -1.5 -1.4 ILE899 IIII(C12)H 3 -1.5 -1.5 -1.5 -1.4 O.9 O.9 AALA877 IIII(C12)H 3 -0.7 -0.7 -0.7 O.7 O.7 VAL746 IIII(C12)H 3 -0.7 -0.7 -0.7 O.7 O.7 VAL746 IIII(C12)H 3 -0.7 -0.5 -0.5 -0.5 PHE891 IIII(C12)H 3.5 -1.1 -0.9 O.9 SER703 IIII(C12)H 3.5 -1.1 -0.9 O.9 SER703 III(C12)H IIIIC13)H 3.5 -0.5 -0.5 -0.5 -0.5 O.5 O.5 O.5 O.5 O.5 O.5 O.5 O.5 O.5 O	Residue	Atomic Group			Energy (ε=20)	Energy (ε=40)	
LEU707		. , . , , ,					
GLN711							
MET745							
PHE764   III(C7)F; II(C4)N   2.5   0.8   0.9   0.8   0.9							
MET895							
LEU701							
GLY708							
MET742							
MET749   III(C7)F; I(N1)O   3   -3.7   -3.6   -3.6   ARG752   I(N1)O   3   -3.9   -3.3   -3.3   -3.0   MET787   III(C7)F   3   -1.7   -1.7   -1.7   PHE876   III(C13)H   3   -1.0   -1.0   -0.9   ALA877   III(C12)H; III(C12)H   3   -1.5   -1.5   -1.4   ILE899   III(C12)H; III(C12)H   3   -0.7   -0.7   -0.7   VAL746   II(C7)F   3.5   -1.4   -1.4   -1.4   -1.4   MET780   III(C3)H; III(C10)O   3.5   -1.4   -1.3   -1.3   -1.3   LEU873   III(C13)H   3.5   -0							
ARG752							
MET787 III(C7)F 3 -1.7 -1.7 -1.7 PHE876 IIII(C13)H 3 -1.0 -1.0 -1.0 -0.9 ALA877 IIII(C12)H; III(C12)H 3 -1.5 -1.5 -1.4 IILE899 IIII(C12)H; III(C12)H 3 -1.5 -1.4 -1.4 -1.4 IILE899 IIII(C12)H; III(C10)H 3 -0.7 -0.7 -0.7 -0.7 VAL746 III(C7)F 3.5 -1.4 -1.4 -1.4 -1.4 -1.4 -1.4 IILE879 IIII(C3)H; III(C10)O 3.5 -1.4 -1.3 -1.3 -1.3 ILEU873 III(C7)F 3.5 -1.6 -1.6 -1.6 -1.6 -1.6 III(C3)H; III(C12)H 3.5 -0.5 -0.5 -0.5 -0.5 -0.5 -0.5 -0.5 III(C12)H 3.5 -1.1 -0.9 -0.9 SER703 III(C13)H 3.5 -1.1 -0.9 -0.9 SER703 III(C13)H 5 -1.9 -0.3 -0.2 GLU709 III(N1)O; III(C5)H 5 -1.9 -0.3 -0.2 IIII(C12)H; III(C10)H 5 -0.5 -0.5 -0.5 -0.5 IIIIIII(C12)H; IIII(C10)H 5 -0.5 -0.5 -0.5 IIIIIII(C12)H; IIII(C12)H; IIII(C12)H 5 -0.1 -0.1 -0.1 SER702 IIII(C12)H 5 -0.1 -0.1 -0.1 -0.1 SER702 IIIIII(C12)H; IIII(C12)H 5.5 -0.2 -0.2 -0.2 IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII			3				
PHEB76							
ALAB77   III(C12)H; III(C12)H   3			3				
ILE899							
VAL746   II(C3)F   3.5   -1.4   -1.4   -1.4   MET780   III(C3)H; III(C10)O   3.5   -1.4   -1.3   -1.3   LEUB73   III(C13)H   3.5   -1.6   -1.6   -1.6   -1.6   LEUB80   III(C13)H   3.5   -0.5   -0.5   -0.5   PHE891   III(C12)H   3.5   -1.1   -0.9   -0.9   SER703   I(C5)H; I(N1)O   5   0.0   0.0   0.0   GLU706   I(C2)H; I(C5)H   5   -1.9   -0.3   -0.2   GLU709   I(N1)O; I(C5)H   5   -0.4   -0.3   -0.2   TRP741   III(C12)H; I(N1)O   5   -0.5   -0.5   -0.5   CYS784   I(C2)H   5   -0.1   -0.1   -0.1   SER702   I(N1)O   5.5   -0.2   -0.2   -0.1   ALA748   I(N1)O1; I(C5)H   5.5   -0.3   -0.2   -0.2   LEU762   I(C5)H   5.5   -0.2   -0.2   -0.2   TYR763   I(N1)O1; I(C2)H   5.5   -0.2   -0.1   -0.1   VAL889   I(C5)H   5.5   -0.2   -0.1   -0.1   PRO892   I(C2)H; I(C5)H   5.5   -0.1   -0.1   -0.1   LEU700   I(N1)O   6   -0.1   -0.1   -0.1   LEU744   I(C2)H; I(C5)H   6   -0.4   -0.4   -0.4   GLY750   I(N1)O; II(C7)F   6   -0.1   -0.1   -0.1   LEU768   I(C2)H   6   -0.1   -0.1   -0.1   ALA765   I(C2)H   6   -0.1   -0.1   -0.1   ARG710   I(C2)H   6.5   -0.2   -0.2   -0.2   LEU878   II(C2)H; I(C5)H   6.5   -0.1   -0.1   -0.1   ARG710   I(C2)H   6.5   -0.1   -0.1   -0.1   ASP890   I(C2)H; I(C5)H   6.5   -0.1   -0.1   -0.1   ASP890   I(C2)H   6.5   -0.1   -0.1   -0.1   -0.1   ASP890   I(C2)H   6.5   -0.1   -0.1   -0.1   -0.1   ASP890   I(C2)H; I(C5)H   7   -0.1   -							
MET780							
LEU873 II(C7)F 3.5 -1.6 -1.6 -1.6 -1.6 LEU880 III(C13)H 3.5 -0.5 -0.5 -0.5 -0.5 -0.5 PHE891 III(C12)H 3.5 -1.1 -0.9 -0.9 SER703 I(C5)H; I(N1)O 5 0.0 0.0 0.0 0.0 GLU706 I(C2)H; I(C5)H 5 -1.9 -0.3 -0.2 GLU709 I(N1)O; I(C5)H 5 -0.4 -0.3 -0.2 GLU709 II(N1)O; I(C5)H 5 -0.5 -0.5 -0.5 -0.5 -0.5 CYS784 I(C2)H 5 -0.1 -0.1 -0.1 -0.1 SER702 I(N1)O 5.5 -0.5 -0.2 -0.2 -0.1 ALA748 I(N1)O1; I(C5)H 5.5 -0.3 -0.2 -0.2 ILEU762 I(C5)H 5.5 -0.2 -0.2 -0.2 ILEU762 I(C5)H 5.5 -0.2 -0.2 -0.2 INTR763 I(N1)O1; I(C2)H 5.5 -0.2 -0.1 -0.1 -0.1 PRO892 I(C2)H; I(C5)H 5.5 -0.1 -0.1 -0.1 PRO892 I(C2)H; I(C5)H 5.5 -0.1 -0.1 -0.1 -0.1 ILEU700 I(N1)O 6 -0.1 -0.1 -0.1 ILEU744 I(C2)H; I(C5)H 6 -0.4 -0.4 -0.4 GLY750 I(N1)O; II(C7)F 6 -0.1 -0.1 -0.1 ILEU768 I(C2)H; I(C5)H 6.5 -0.2 -0.2 -0.2 ILEU881 I(C2)H; I(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 II(C2)H; I(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 II(C2)H; I(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 III(C2)H; III(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 III(C2)H; III(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 IIII(C2)H; III(C5)H 6.5 -0.1 -0.1 -0.1 ILEU768 IIII(C2)H; IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII							
LEU880         III(C13)H         3.5         -0.5         -0.5         -0.5           PHE891         III(C12)H         3.5         -1.1         -0.9         -0.9         -0.9           SER703         I(C5)H; I(N1)O         5         0.0         0.0         0.0           GLU706         I(C2)H; I(C5)H         5         -1.9         -0.3         -0.2           GLU709         I(N1)O; I(C5)H         5         -0.4         -0.3         -0.2           TRP741         III(C12)H; I(N1)O         5         -0.5         -0.5         -0.5         -0.5           CYS784         I(C2)H         5         -0.1         -0.1         -0.1         -0.1           SER702         I(N1)O; I(C5)H         5.5         -0.2         -0.2         -0.1         -0.1           ALA748         I(N1)O1; I(C2)H         5.5         -0.3         -0.2							
PHE891							
SER703         I(C5)H; I(N1)O         5         0.0         0.0         0.0           GLU706         I(C2)H; I(C5)H         5         -1.9         -0.3         -0.2           GLU709         I(N1)O; I(C5)H         5         -0.4         -0.3         -0.2           TRP741         IIII(C12)H; I(N1)O         5         -0.5         -0.5         -0.5           CYS784         I(C2)H         5         -0.1         -0.1         -0.1           SER702         I(N1)O         5.5         -0.2         -0.2         -0.1           ALA748         I(N1)O1; I(C5)H         5.5         -0.3         -0.2         -0.2           LEU762         I(C5)H         5.5         -0.2         -0.2         -0.2           TYR763         I(N1)O1; I(C2)H         5.5         -0.2         -0.2         -0.2           TYR763         I(N1)O1; I(C2)H         5.5         -0.2         -0.1         -0.1           VAL889         I(C5)H         5.5         -0.2         -0.1         -0.1           VAL889         I(C2)H; I(C5)H         5.5         -0.1         -0.1         -0.1           LEU700         I(N1)O; II(C5)H         6         -0.1         -0.1         <							
GLU706							
GLU709   I(N1)O; I(C5)H   5							
TRP741   III(C12)H; I(N1)O							
CYS784							
SER702         I(N1)O         5.5         -0.2         -0.2         -0.1           ALA748         I(N1)O1; I(C5)H         5.5         -0.3         -0.2         -0.2           LEU762         I(C5)H         5.5         -0.2         -0.2         -0.2           TYR763         I(N1)O1; I(C2)H         5.5         -0.2         -0.1         -0.1           VAL889         I(C5)H         5.5         -0.1         -0.1         -0.1           PRO892         I(C2)H; I(C5)H         5.5         -0.1         -0.1         -0.1           LEU700         I(N1)O         6         -0.1         -0.1         -0.1           LEU744         I(C2)H; I(C5)H         6         -0.4         -0.4         -0.4           GLY750         I(N1)O; II(C7)F         6         -0.1         -0.1         -0.0           ALA765         I(C2)H         6         -0.1         -0.1         -0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C3)H; I(C5)H         6.5         -0.1         -0.1         -0.1 </td <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>							
ALA748							
LEU762							
TYR763							
VAL889         I(C5)H         5.5         -0.1         -0.1         -0.1           PRO892         I(C2)H; I(C5)H         5.5         -0.1         -0.1         -0.1           LEU700         I(N1)O         6         -0.1         -0.1         -0.1           LEU744         I(C2)H; I(C5)H         6         -0.4         -0.4         -0.4           GLY750         I(N1)O; II(C7)F         6         -0.1         0.0         0.0           ALA765         I(C2)H         6         -0.1         -0.1         0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         II(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1							
PRO892							
LEU700         I(N1)O         6         -0.1         -0.1         -0.1           LEU744         I(C2)H; I(C5)H         6         -0.4         -0.4         -0.4           GLY750         I(N1)O; II(C7)F         6         -0.1         0.0         0.0           ALA765         I(C2)H         6         -0.1         -0.1         0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         -0.1         -0.1							
LEU744         I(C2)H; I(C5)H         6         -0.4         -0.4         -0.4           GLY750         I(N1)O; II(C7)F         6         -0.1         0.0         0.0           ALA765         I(C2)H         6         -0.1         -0.1         0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1							
GLY750         I(N1)O; II(C7)F         6         -0.1         0.0         0.0           ALA765         I(C2)H         6         -0.1         -0.1         0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         -0.1         -0.1           VAL715         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           VAL715         I(C5)H; I(C7)F         7         0.0         0.0         0.0 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>							
ALA765         I(C2)H         6         -0.1         -0.1         0.0           LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         II(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         -0.1         -0.1           VAL687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H; I(C7)F         7         -0.1         -0.1         -0.1           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0							
LEU768         I(C2)H; I(N1)O         6         -0.2         -0.2         -0.2           LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         II(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           SER753         II(C7)F; I(N1)O         7         -0.1         0.0         0.0							
LEU881         I(C2)H         6         -0.1         -0.1         -0.1           ARG710         I(C2)H         6.5         0.2         0.0         0.0           PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H; I(C7)F         7         0.0         0.0         0.0           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           SER753         II(C7)F; I(N1)O         7         -0.1         0.0         0.0							
ARG710							
PHE747         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H         7         -0.1         -0.1         0.0           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           GLY743         II(C7)F         7         0.0         0.0         0.0           SER753         III(C7)F; I(N1)O         7         -0.1         0.0         0.0			_				
GLN783         I(N1)O; I(C2)H         6.5         -0.1         -0.1         -0.1           HIS874         I(C2)H; I(C5)H         6.5         -0.1         -0.1         -0.1           PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H         7         -0.1         -0.1         0.0           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           GLY743         II(C7)F         7         0.0         0.0         0.0           SER753         II(C7)F; I(N1)O         7         -0.1         0.0         0.0							
HIS874 I(C2)H; I(C5)H 6.5 -0.1 -0.1 -0.1 PHE878 III(C12)H 6.5 -0.1 -0.1 -0.1 ASP890 I(C2)H 6.5 -0.4 -0.2 -0.1 VAL685 I(N1)O; I(C5)H 7 -0.1 0.0 0.0 ALA687 I(C5)H; I(C6)H 7 -0.1 -0.1 -0.1 LEU712 I(C5)H 7 -0.1 -0.1 0.0 VAL715 I(C5)H; II(C7)F 7 0.0 0.0 0.0 GLY743 II(C7)F; I(N1)O 7 -0.1 0.0 0.0 SER753 II(C7)F; I(N1)O 7 -0.1 0.0							
PHE878         III(C12)H         6.5         -0.1         -0.1         -0.1           ASP890         I(C2)H         6.5         -0.4         -0.2         -0.1           VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H         7         -0.1         -0.1         0.0           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           GLY743         II(C7)F         7         0.0         0.0         0.0           SER753         II(C7)F; I(N1)O         7         -0.1         0.0         0.0							
ASP890 I(C2)H 6.5 -0.4 -0.2 -0.1 VAL685 I(N1)O; I(C5)H 7 -0.1 0.0 0.0 ALA687 I(C5)H; I(C6)H 7 -0.1 -0.1 -0.1 LEU712 I(C5)H 7 -0.1 -0.1 0.0 VAL715 I(C5)H; II(C7)F 7 0.0 0.0 0.0 GLY743 II(C7)F 7 0.0 0.0 0.0 SER753 II(C7)F; I(N1)O 7 -0.1 0.0							
VAL685         I(N1)O; I(C5)H         7         -0.1         0.0         0.0           ALA687         I(C5)H; I(C6)H         7         -0.1         -0.1         -0.1           LEU712         I(C5)H         7         -0.1         -0.1         0.0           VAL715         I(C5)H; II(C7)F         7         0.0         0.0         0.0           GLY743         II(C7)F         7         0.0         0.0         0.0           SER753         II(C7)F; I(N1)O         7         -0.1         0.0         0.0							
ALA687       I(C5)H; I(C6)H       7       -0.1       -0.1       -0.1         LEU712       I(C5)H       7       -0.1       -0.1       0.0         VAL715       I(C5)H; II(C7)F       7       0.0       0.0       0.0         GLY743       II(C7)F       7       0.0       0.0       0.0         SER753       II(C7)F; I(N1)O       7       -0.1       0.0       0.0							
LEU712       I(C5)H       7       -0.1       -0.1       0.0         VAL715       I(C5)H; II(C7)F       7       0.0       0.0       0.0         GLY743       II(C7)F       7       0.0       0.0       0.0         SER753       II(C7)F; I(N1)O       7       -0.1       0.0       0.0							
VAL715       I(C5)H; II(C7)F       7       0.0       0.0       0.0         GLY743       II(C7)F       7       0.0       0.0       0.0         SER753       II(C7)F; I(N1)O       7       -0.1       0.0       0.0							
GLY743 II(C7)F 7 0.0 0.0 0.0 SER753 II(C7)F; I(N1)O 7 -0.1 0.0 0.0							
SER753 II(C7)F; I(N1)O 7 -0.1 0.0 0.0							
<b>\</b>	PHE770	III(C13)H	7	-0.2	-0.2	-0.2	
SER778 III(C13)H 7 -0.1 -0.1 -0.1							
ILE869 II(C7)F 7 -0.1 -0.1 -0.1	ILE869	II(C7)F	7	-0.1	-0.1	-0.1	

ALA870	II(C7)F	7	0.0	0.0	0.0
ALA896	III(C12)H	7	0.0	0.0	0.0
VAL903	III(C12)H	7	0.0	0.0	0.0
	, ,				
PHE697	III(C13)H	7.5	-0.1	-0.1	-0.1
LEU790	II(C7)F	8	-0.1	0.0	0.0
GLN875	I(C6)H; III(C13)H	8	-0.1	-0.1	0.0
ASP879	III(C12)H; III(C13)H	8	-0.1	-0.1	0.0
SER884	III(C13)H; III(C12)H	8	0.0	0.0	0.0
ILE898	III(C12)H	8	0.0	0.0	0.0
CYS686	I(C5)H	8.5	0.0	0.0	0.0
ALA698	III(C13)H	8.5	-0.1	0.0	0.0
ALA699	III(O11)H	8.5	-0.1	0.0	0.0
PRO766	I(N1)O	8.5	0.0	0.0	0.0
VAL866	II(C7)F	8.5	0.0	0.0	0.0
GLU872	III(C10)O; III(C13)H	8.5	0.0	0.0	0.0
VAL887	III(C13)H	8.5	0.0	0.0	0.0
MET894	III(C12)H	8.5	0.0	0.0	0.0
HIS714	I(C5)H; I(N1)O	9	0.0	0.0	0.0
TRP751	IÌ(C7)F; I(N1)O	9	-0.1	-0.1	0.0
VAL769	I(N1)O	9	0.0	0.0	0.0
MET775	II(C7)F	9	-2.0	0.0	0.0
ARG779	III(C13)C	9	0.1	0.0	0.0
ILE882	III(C13)H; III(C12)H	9	0.0	0.0	0.0
SER900	III(C12)H	9	0.0	0.0	0.0
HIS689	I(C6)H	9.5	0.0	0.0	0.0
VAL713	I(C5)H	9.5	0.0	0.0	0.0
SER740	II(C7)F	9.5	0.0	0.0	0.0
ASP767	I(C5)H	9.5	-0.1	-0.1	0.0
ARG786	IÌ(C႗)F	9.5	-0.2	-0.1	-0.1
ARG788	II(C7)F	9.5	-0.1	-0.1	0.0
SER791	II(C7)F	9.5	0.0	0.0	0.0
LYS808	I(N1)O	9.5	-0.2	-0.1	-0.1
LYS883	III(C13)H	9.5	0.1	-0.4	0.0
GLU897	III(C12)H	9.5	-0.1	-0.1	0.0
PRO682	I(N1)O	10	0.3	0.0	0.0
VAL785	II(C7)F	10	0.3	0.0	0.0
PHE804	I(N1)O	10	0.3	0.0	0.0
ARG871	III(C10)O; III(C12)H	10	0.5	-0.1	0.0
GLU893	III(C12)H	10	-0.2	-0.1	0.0
GLY683	I(N1)O	10.5	0.0	0.0	0.0
VAL684	I(N1)O	10.5	0.0	0.0	0.0
GLY688	I(C6)H; I(C5)H	10.5	0.0	0.0	0.0
GLN738	III(C12)H	10.5	0.0	0.0	0.0
MET761	II(C7)F	10.5	0.0	0.0	0.0
ARG774					
	III(C13)H	10.5	0.0	0.0	0.0
TYR781	III(C13)H	10.5	0.0	0.0	0.0
SER782	II(C7)F	10.5	0.0	0.0	0.0
LEU811	II(C7)F	10.5	0.0	0.0	0.0
LEU907	III(C12)H; III(C13)H	10.5	0.0	0.0	0.0
PHE754	II(C7)F; I(N1)O	11	0.0	0.0	0.0
LYS777	III(C13)H	11	0.1	0.0	0.0
PHE794	II(C7)F; I(N1)O	11	0.0	0.0	0.0
GLN867	II(C7)F	11	0.0	0.0	0.0
SER888	III(C13)H	11	0.0	0.0	0.0
GLN902	III(C12)H	11	0.0	0.0	0.0
GLINDUZ	111(012)11	1.1	0.0	0.0	0.0

PRO904	III(C12)H	11	0.0	0.0	0.0
ILE906	III(C12)H	11	0.0	0.0	0.0

TABLE S3. RLL interaction in complex with the AR receptor, regions and groups where there is drug-residue interaction, radius and energetic value (in kcal/mol).

		Complex A	AR-RLL		
Residue	Atomic Group	r (Å)	Energy (ε=10)	Energy (ε=20)	Energy (ε=40)
LEU701	II(C12)H	2.5	-1.9	-1.8	-1.7
LEU704	III(C1)H	2.5	-0.9	-0.8	-0.7
ASN705	II(OH)H	2.5	-11.2	-5.2	-5.1
LEU707	III(C2)H	2.5	-2.1	-2.1	-2.1
GLN711	III(C2)H	2.5	0.1	0.0	-0.1
TRP741	II(CAQ)H; I(CAK)H	2.5	-4.6	-4.4	-4.3
MET742	I(CAK)H	2.5	-4.4	-4.2	-4.1
MET745	I(CAK)H	2.5	-3.2	-3.2	-3.0
ARG752 PHE764	III(C8)N	2.5	-1.9	-1.9	-1.7
ILE899	IV(C7)F I(C21)H	2.5 2.5	-3.1 -2.0	-3.1 -2.0	-3.1 -2.0
GLY708	I(CAR)H; III(C1)H		-2.0 -2.5	-2.0 -2.4	
MET749	I(CAR)H, III(CT)H IV(C7)F	3 3	-2.5 -2.8	-2.4 -2.8	-2.3 -2.6
MET780	II(C12)H	3	-2.6 -2.3	-2.6 -2.2	-2.0 -2.2
PHE876	II(C12)H	3	-2.3 -1.3	-2.2 -1.3	-2.2 -1.3
ALA877	I(C21)H	3	-1.9	-1.9	-1.9
MET895	I(C16)O	3	-1.9 -4.9	-1. <del>9</del> -4.7	-1. <del>9</del> -4.6
VAL746	IV(C7)F	3.5	-4.9 -2.0	-4.7 -1.9	-4.0 -0.9
MET787	IV(C7)F	3.5	-1.6	-1.6	-0.3
LEU873	IV(C7)F	3.5	-2.3	-2.3	-2.2
LEU880	II(C12)H	3.5	-0.6	-0.6	-0.5
ILE898	I(C22)N	3.5	-3.1	-0.7	0.0
HIS874	I(C20)H	4	-1.2	-1.2	-1.3
PHE891	II(C3)H; I(C21)H	4	-0.8	-0.2	-0.7
VAL903	I(C22)N	4	-0.9	-0.9	-0.9
GLN738	I(C22)N	4.5	-0.4	-0.3	-0.1
SER703	III(C1)H	5	-0.6	-0.6	-0.6
VAL715	I(CAK)H	5	-0.1	-0.1	-0.1
TYR763	III(C8)N	5	-0.2	-0.3	-0.2
LEU768	III(C1)H	5	-0.3	-0.3	-0.3
GLU706	II(OH)H	5.5	-0.7	-0.4	-0.2
GLU709	IIÌ(C1)H	5.5	-0.7	-0.4	-0.4
GLY743	II(CAQ)H; Í(CAK)H	5.5	-0.2	-0.2	-0.2
LEU744	I(CAK)H	5.5	-0.2	-0.2	-0.2
ALA748	IÌI(C8)N	5.5	-0.4	-0.3	-0.3
LEU762	IV(C7)F	5.5	-0.3	-0.3	-0.2
ALA765	III(C2)H	5.5	0.1	0.1	0.1
VAL889	II(C12)H	5.5	0.3	0.1	0.0
GLN902	I(C22)N	5.5	-0.2	-0.2	-0.1
ALA687	III(C1)H; III(C2)H	6	-0.1	-0.1	-0.1
LEU700	II(OH)H	6	-0.1	-0.1	-0.1
SER702	II(OH)H	6	-0.2	0.1	-0.1
LEU712	I(CAK)H	6	-0.3	-0.3	-0.3
TYR739	I(C22)N	6	-0.1	-0.1	0.0
SER740	II(CAQ)H; I(CAK)H	6	-0.1	0.0	0.0
PHE747	IV(C7)F	6	-0.1	-0.1	-0.1
GLY750	IV(C7)F	6	0.0	0.0	0.0
SER778	II(C12)H	6	-0.1	-0.1	-0.1
CYS784	IV(C7)F	6	-0.1	-0.1	-0.1
PHE878	I(C21)H; I(C20)H	6	-0.2	-0.1	-0.1
PRO892	II(OH)H	6	-0.2	-0.2	-0.1
ILE906	I(C22)N	6	-0.1	-0.1	-0.1
ILE737	I(C22)N; II(CAQ)H	6.5	0.0	0.0	-0.1

PHE770	II(C12)H	6.5	-0.2	-0.2	-0.2
ALA870	IV(C7)F	6.5	-0.1	-0.1	-0.1
LEU881	I(C21)H	6.5	0.2	-0.1	-0.1
VAL685	III(C2)H	7	-0.1	-0.1	-0.1
PHE697	II(C12)H	7	-0.1	-0.1	-0.1
ARG710	III(C1)H; III(C2)H	7	0.3	0.1	0.0
SER753	IV(C7)F	7	-0.1	-0.1	0.0
GLN783	IV(C7)F	7	-0.1	-0.1	-0.1
ILE869	IV(C7)F	7	-0.1	-0.1	-0.1
ASP890	II(OH)H	7	-0.5	-0.2	-0.1
ALA896	I(C21)H; I(C20)H	7	0.0	0.0	0.0
MET894	I(C20)H	7.5	-0.8	-0.1	-0.1
SER900	I(C20)H	7.5	0.0	0.0	0.0
CYS686	III(C2)H	8	0.0	0.0	0.0
PRO766	III(C2)H; III(C8)N	8	0.0	0.0	0.0
LEU790	IV(C7)F	8	0.0	0.0	0.0
ILE815	I(C22)N	8	0.0	0.0	0.0
GLU872	II(C12)H	8	-0.1	-0.1	-0.1
GLN875	I(C20)H; II(C3)H	8	-0.1	-0.1	-0.1
PRO904	I(C22)N; I(C20)H	8	0.0	0.0	0.0
HIS689	III(C1)H	8.5	0.0	0.0	0.0
ALA699	II(OH)H	8.5	-0.3	-0.1	0.0
TRP751	IV(C7)F; III(C8)N	8.5	-0.1	-0.1	-0.1
ARG779	II(C12)H	8.5	0.1	0.0	0.0
VAL866	IV(C7)F	8.5	0.0	0.0	0.0
VAL887	II(C12)H	8.5	0.0	0.0	0.0
GLU897	I(C22)N	8.5	-0.1	-0.1	0.0
VAL901	I(C22)N; I(C20)H	8.5	-0.1	-0.1	0.0
LEU907	I(C22)N; I(C20)H	8.5	0.0	0.0	0.0
ALA698	II(OH)H	9	-0.1	0.0	0.0
VAL713	I(CAK)H	9	0.0	0.0	0.0
ALA735	I(C22)N	9	0.1	0.0	0.0
VAL736	I(C22)N	9	0.0	0.0	0.0
ASP767	III(C2)H	9	-0.3	-0.2	-0.1
VAL769	III(C8)N	9	-0.1	0.0	0.0
ARG788	IV(C7)F	9	0.0	0.0	0.0
SER791	IV(C7)F	9	0.0	0.0	0.0
ARG871	I(C22)N	9	-0.1	-0.1	-0.1
ASP879	II(C13)H	9	-0.1	-0.1	0.0
SER884	II(C3)H; II(C12)H	9	0.0	0.0	0.0
VAL684	III(C8)N	9.5	0.0	0.0	0.0
GLY688	III(C1)H; III(C2)H	9.5	0.0	0.0	0.0
HIS714	III(C2)H	9.5	0.0	0.0	0.0
VAL716	I(CAK)H; II(CAQ)H	9.5	0.0	0.0	0.0
ASN756	III(C8)N	9.5	0.0	0.0	0.0
ARG774	II(C12)H	9.5	0.1	0.0	0.0
MET775	II(C12)H; IV(C7)F	9.5	0.0	0.0	0.0
ARG786	IV(C7)F	9.5	-0.2	-0.1	-0.1
LEU811	I(CAK)H	9.5	0.0	0.0	0.0
LYS883	II(C12)H	9.5	0.2	0.1	0.0
TRP718	I(CAK)H	10	0.0	0.0	0.0
MET734	I(C22)N	10	0.0	0.0	0.0
MET761	IV(C7)F	10	0.0	0.0	0.0
LYS777	II(C12)H	10	0.1	0.1	0.0
TYR781	II(C12)H	10	0.0	0.0	0.0

VAL785	IV(C7)F	10	0.0	0.0	0.0
PHE804	III(C8)N	10	0.0	0.0	0.0
LYS808	III(C8)N; IV(C7)F	10	-0.1	-0.1	0.0
LEU812	I(CAK)H	10	0.0	0.0	0.0
ILE882	I(C20)H; II(C3)H	10	0.0	0.0	0.0
GLU893	I(C21)H	10	-0.1	-0.1	0.0
LYS905	I(C22)N	10	-0.3	-0.2	-0.1
VAL911	I(C22)N	10	0.0	0.0	0.0
PRO682	III(C8)N	10.5	0.0	0.0	0.0
GLY683	III(C8)N	10.5	0.0	0.0	0.0
SER696	II(C12)H	10.5	0.0	0.0	0.0
PHE754	III(C8)N	10.5	0.0	0.0	0.0
PHE794	IV(C7)F	10.5	0.0	0.0	0.0
GLN867	II(CAQ)H; IV(C7)F	10.5	0.0	0.0	0.0
ALA719	I(CAK)H	11	0.0	0.0	0.0
SER782	II(C12)H	11	0.0	0.0	0.0
HIS789	IV(C7)F	11	0.0	0.0	0.0
PRO868	IV(C7)F	11	0.0	0.0	0.0
SER888	II(OH)F; II(C12)H	11	0.0	0.0	0.0