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).

Complex AR-CPA					
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	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	0.9	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	-3.7	-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	-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
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	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
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
GLN783	III(C15)H	6	-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

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	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	III(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	I(C3)O	10.5	0.0	0.0	0.0
LEU811	I(C4)H	10.5	0.0	0.0	0.0
PRO868	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).

Complex AR-HFT					
Residue	Atomic Group	*r* (Å)	Energy (ε=10)	Energy (ε=20)	Energy (ε=40)
LEU704	III(O11)H; (N11)H	2.5	-6.7	-6.0	-5.2
ASN705	III(C11)O	2.5	2.8	3.0	3.2
LEU707	I(C5)H	2.5	-1.7	-1.6	-1.6
GLN711	I(C5)H	2.5	-0.5	-0.5	-0.5
MET745	I(C4)N; I(N1)O	2.5	-0.8	-0.8	-0.8
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
LEU701	III(C13)H; III(C13)H	3	-1.9	-1.8	-1.7
GLY708	III(N8)H	3	-1.9	-1.8	-1.8
MET742	III(C12)H	3	-1.7	-1.7	-1.6
MET749	II(C7)F; I(N1)O	3	-3.7	-3.6	-3.6
ARG752	I(N1)O	3	-3.9	-3.3	-3.0
MET787	II(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
MET780	III(C3)H; III(C10)O	3.5	-1.4	-1.3	-1.3
LEU873	II(C7)F	3.5	-1.6	-1.6	-1.6
LEU880	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	-0.1	-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	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
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

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	II(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	II(C7)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

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 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	III(C8)N	2.5	-1.9	-1.9	-1.7
PHE764	IV(C7)F	2.5	-3.1	-3.1	-3.1
ILE899	I(C21)H	2.5	-2.0	-2.0	-2.0
GLY708	I(CAR)H; III(C1)H	3	-2.5	-2.4	-2.3
MET749	IV(C7)F	3	-2.8	-2.8	-2.6
MET780	II(C12)H	3	-2.3	-2.2	-2.2
PHE876	II(C12)H	3	-1.3	-1.3	-1.3
ALA877	I(C21)H	3	-1.9	-1.9	-1.9
MET895	I(C16)O	3	-4.9	-4.7	-4.6
VAL746	IV(C7)F	3.5	-2.0	-1.9	-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	III(C1)H	5.5	-0.7	-0.4	-0.4
GLY743	II(CAQ)H; I(CAK)H	5.5	-0.2	-0.2	-0.2
LEU744	I(CAK)H	5.5	-0.2	-0.2	-0.2
ALA748	III(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