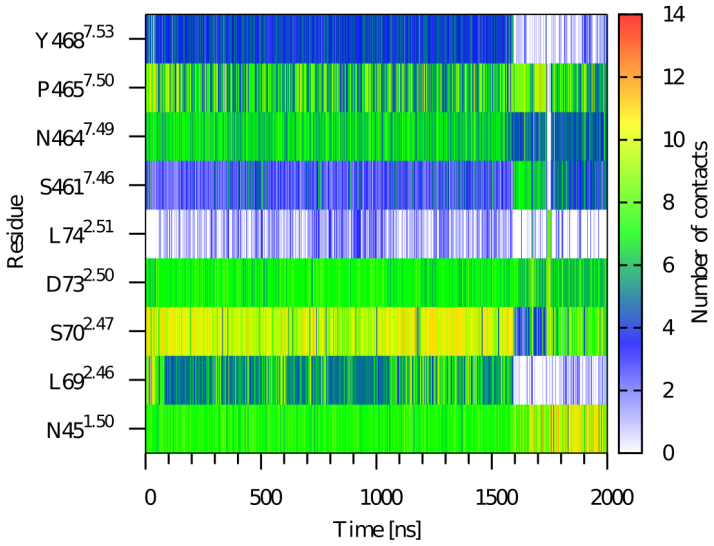
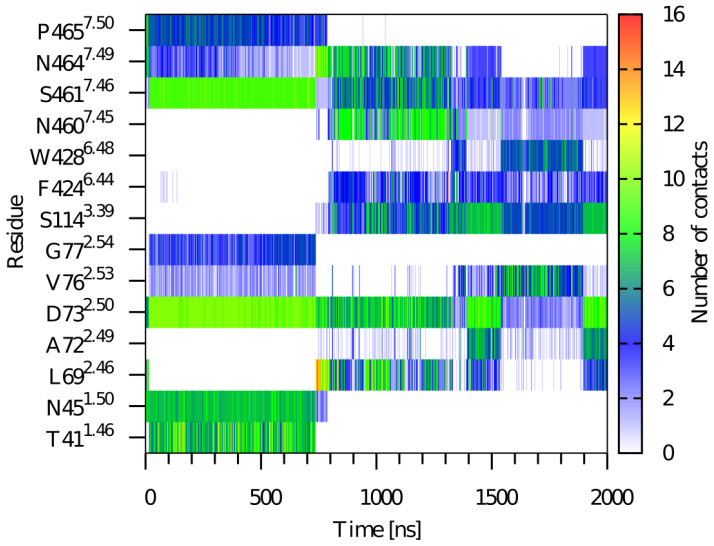
Supplementary Material: Effect of ions and sequence variants on the antagonist binding properties of the histamine H_1 receptor

Marcus Conrad [1], Christian A. Söldner [1] and Heinrich Sticht [1,2]*

A



B



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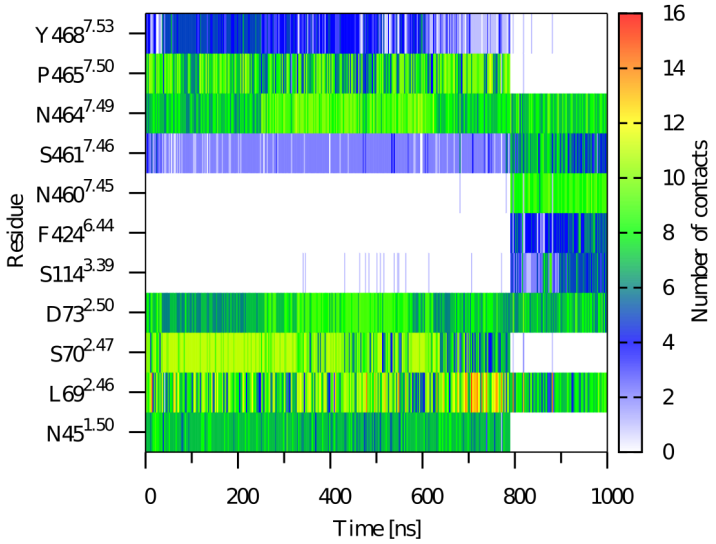
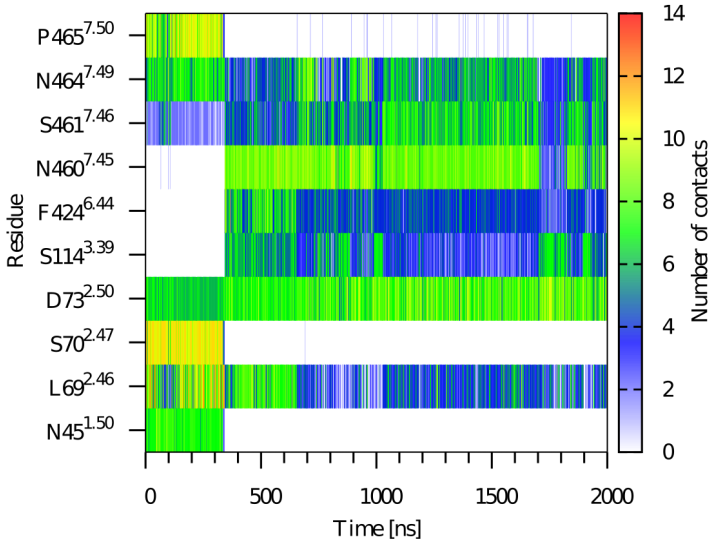
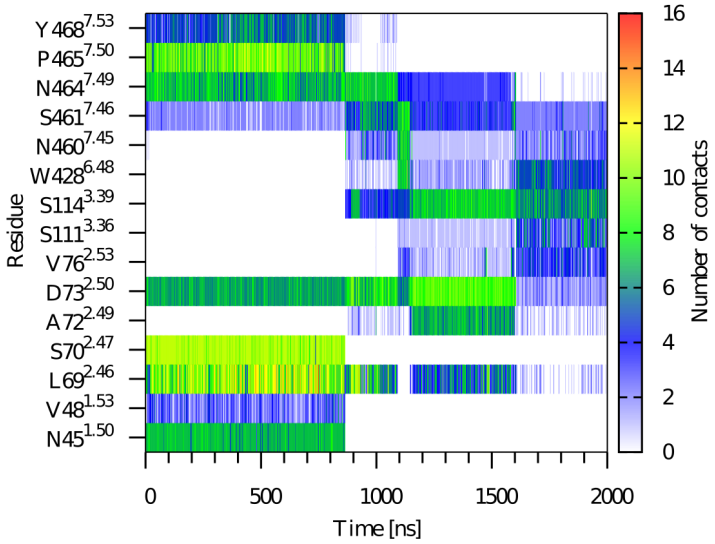

Y468^7.53
P465^7.50
N464^7.49
S461^7.46
N460^7.45
F424^6.44
S114^3.39
D73^2.50
S70^2.47
L69^2.46
N45^1.50
Residue
0
200
400
600
800
1000
Time [ns]
16
14
12
10
8
6
4
2
0
Number of contacts

D


P465^7.50
N464^7.49
S461^7.46
N460^7.45
F424^6.44
S114^3.39
D73^2.50
S70^2.47
L69^2.46
N45^1.50
Residue
0
500
1000
1500
2000
Time [ns]
14
12
10
8
6
4
2
0
Number of contacts

E



F

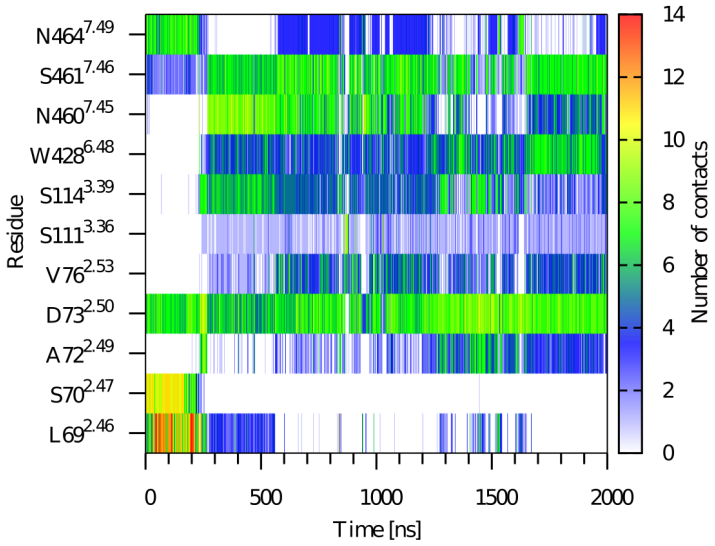
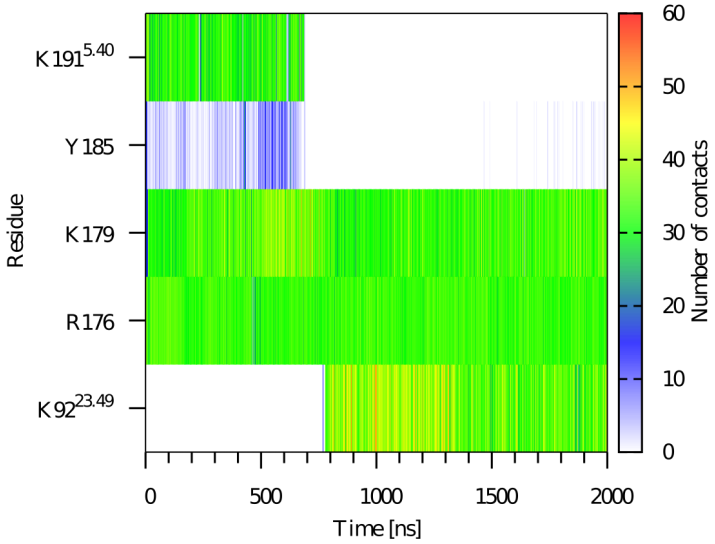
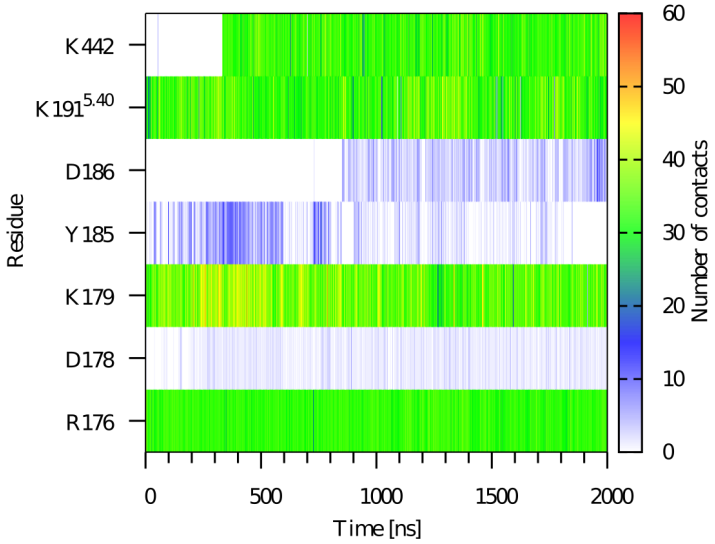


Figure S1. Sodium Interactions Number of contacts between Na+ and H_1R over the simulation time. The simulation time is shown as horizontal axis and the interacting H_1R residues on the vertical axis. The number of contacts is color coded according to the scale shown on the right side of each panel. The Panels A-F represent the runs 1-4,9,10 found in Table 3 (main document).

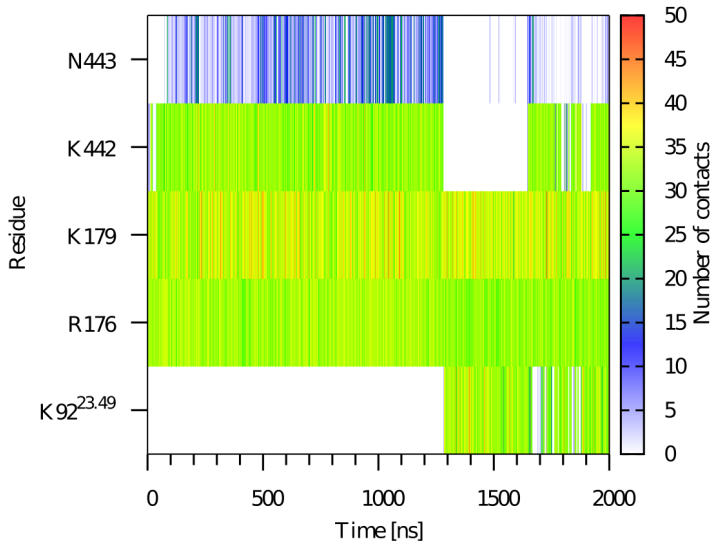
A


K 191 5.40
Y 185
K 179
R 176
K 92 23.49
Residue
0
500
1000
1500
2000
Time [ns]
60
50
40
30
20
10
0
Number of contacts

B


K 442
K 191 5.40
D 186
Y 185
K 179
D 178
R 176
Residue
0
500
1000
1500
2000
Time [ns]
60
50
40
30
20
10
0
Number of contacts

C



D

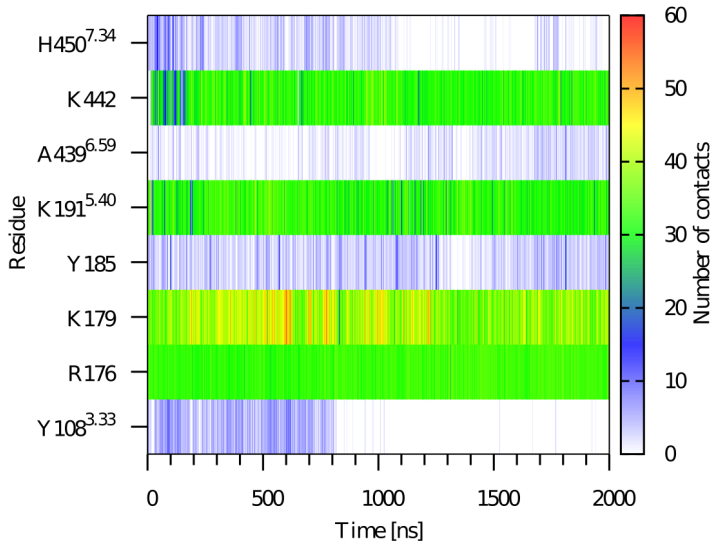
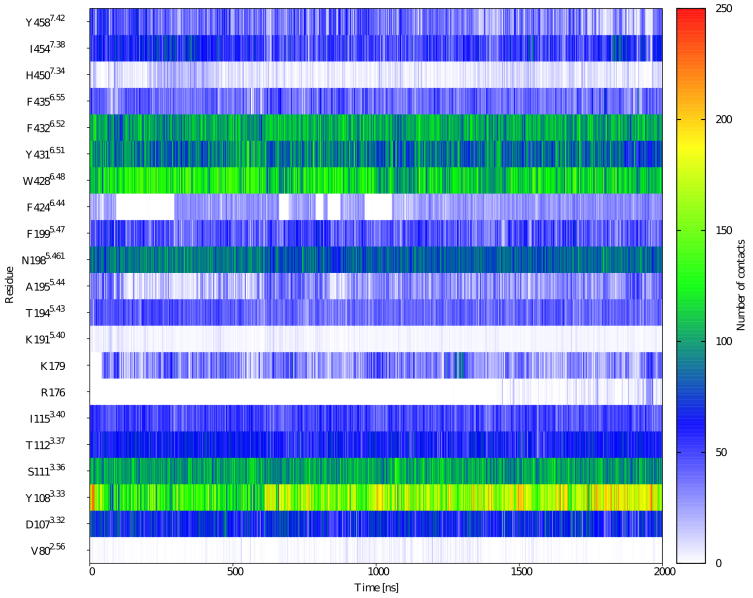
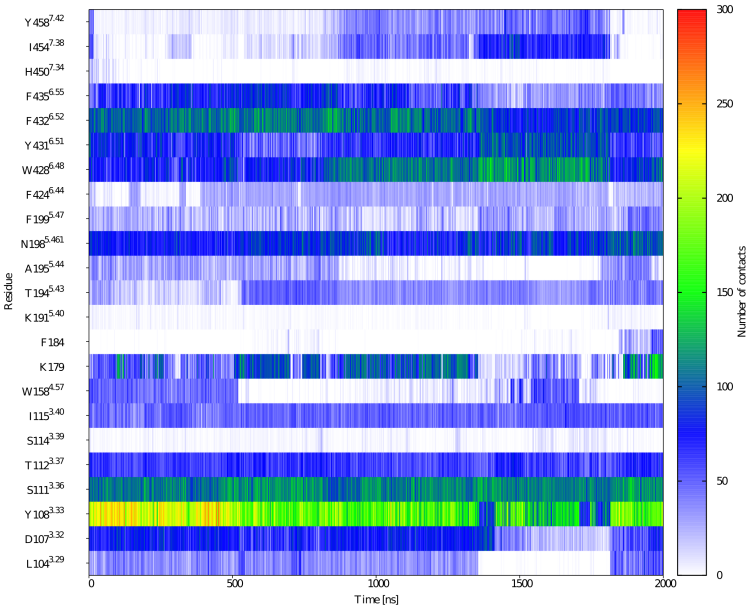


Figure S2. Phosphate Interactions Number of contacts between phosphate ion and H_1R over the simulation time. The simulation time is shown as horizontal axis and the interacting H_1R residues on the vertical axis. The number of contacts is color coded according to the scale shown on the right side of each panel. The Panels A-D represent the runs 3,4,7,8 found in Table 3 (main document).

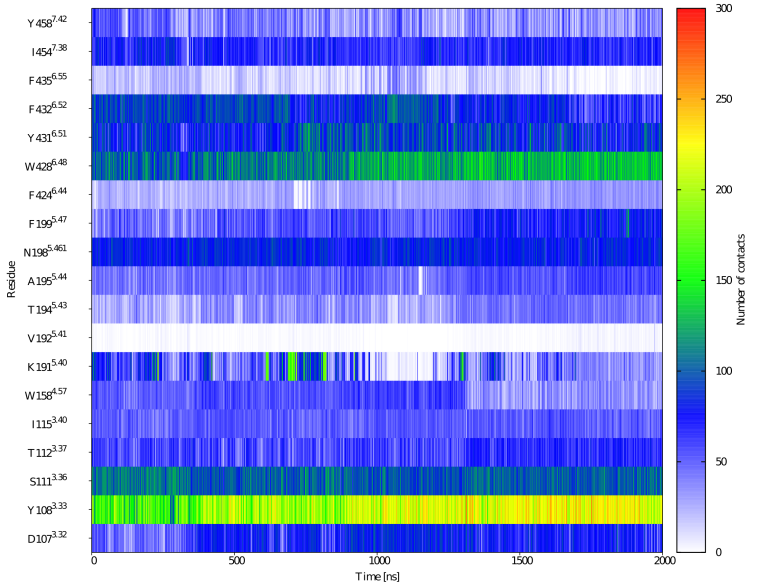
A


Y458^7.42
I454^7.38
H450^7.34
F435^6.55
F432^6.52
Y431^6.51
W428^6.48
F424^6.44
F199^5.47
N196^5.461
A195^5.44
T194^5.43
K191^5.40
K179
R176
I115^3.40
T112^3.37
S111^3.36
Y108^3.33
D107^3.32
V80^2.56
Residue
0
500
1000
1500
2000
Time [ns]
250
200
150
100
50
0
Number of contacts

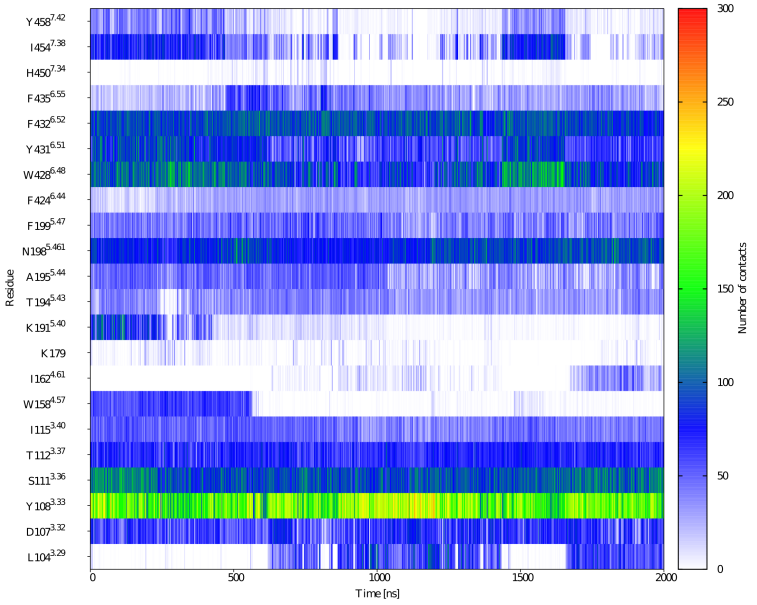
B


Y458^7.42
I454^7.38
H450^7.34
F435^6.55
F432^6.52
Y431^6.51
W428^6.48
F424^6.44
F199^5.47
N196^5.461
A195^5.44
T194^5.43
K191^5.40
F184
K179
W158^4.57
I115^3.40
S114^3.39
T112^3.37
S111^3.36
Y108^3.33
D107^3.32
L104^3.29
Residue
0
500
1000
1500
2000
Time [ns]
300
250
200
150
100
50
0
Number of contacts

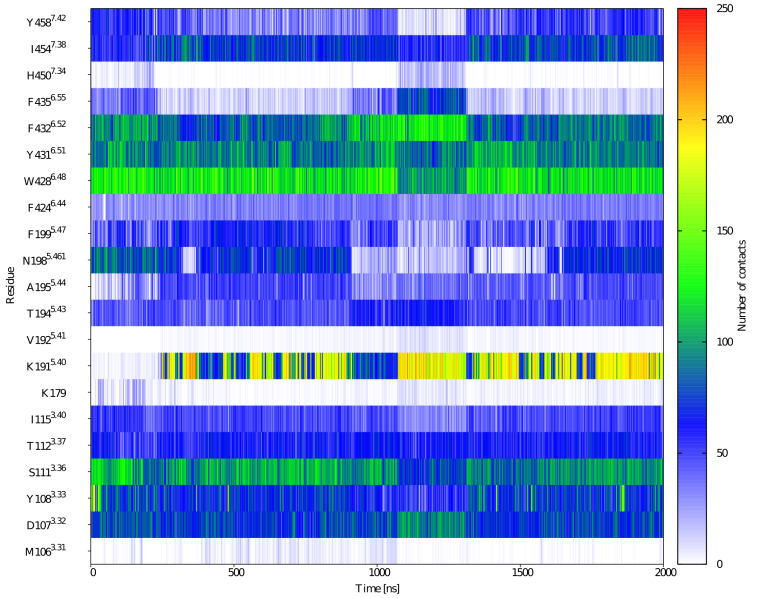
C


Y458^7.42
I454^7.38
F435^6.55
F432^6.52
Y431^6.51
W428^6.48
F424^6.44
F199^5.47
N198^5.461
A195^5.44
T194^5.43
V192^5.41
K191^5.40
W158^4.57
I115^3.40
T112^3.37
S111^3.36
Y108^3.33
D107^3.32
Residue
0
500
1000
1500
2000
Time [ns]
300
250
200
150
100
50
0
Number of contacts

D


Y458^7.42
I454^7.38
H450^7.34
F435^6.55
F432^6.52
Y431^6.51
W428^6.48
F424^6.44
F199^5.47
N198^5.461
A195^5.44
T194^5.43
K191^5.40
K179
I162^4.61
W158^4.57
I115^3.40
T112^3.37
S111^3.36
Y108^3.33
D107^3.32
L104^3.29
Residue
0
500
1000
1500
2000
Time [ns]
300
250
200
150
100
50
0
Number of contacts

E



F

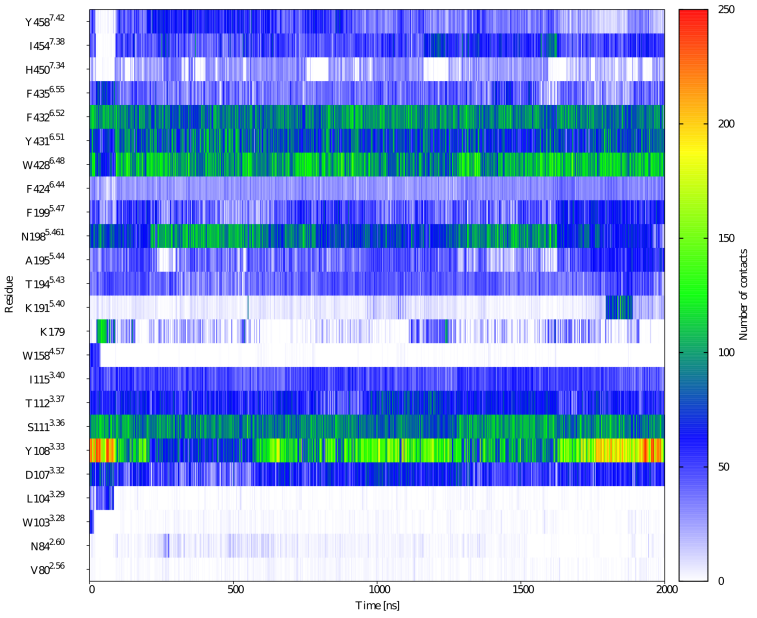


Figure S3. Doxepin Interactions Number of contacts between doxepin and H_1R over the simulation time. The simulation time is shown as horizontal axis and the interacting H_1R residues on the vertical axis. The number of contacts is color coded according to the scale shown on the right side of each panel. The Panels A-F represent the runs1-6 found in Table 3 (main document).