

Glutamate carboxypeptidase II as a model system for designing host-guest units: A theoretical approach

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Theoretical methods

The interaction energies of all complexes used were calculated at the B3LYP¹-D3²/def2-TZVP³ level of theory. The calculations have been performed by using the program TURBOMOLE version 7.0.⁴ The interaction energy values (ΔE) gathered in Tables 1 and 2 were calculated as the energy difference between the complex and the isolated monomers following the supermolecule approximation ($\Delta E_{\text{complex}} = E_{\text{complex}} - E_{\text{monomer1}} - E_{\text{monomer2}}$, see also Figures S1 and S2). In the case of complexes **5** to **14**, the optimization was carried out imposing the C2v symmetry point group to keep the salt bridge interactions in place. In case of calculations regarding PDB structures, the H atoms were initially optimized at the B3LYP-D3/def2-SVP³ level of theory. These geometries were taken as starting points for single point calculations using the def2-TZVP basis set. The MEP (Molecular Electrostatic Potential) surfaces were computed at the B3LYP/def2-TZVP level of theory by means of the Gaussian 16 calculation package. The Bader's "Atoms in molecules" theory has been used to study the interactions discussed herein by means of the AIMall calculation package.⁵ The calculations for the wavefunction analysis have been carried out at the B3LYP/def2-TZVP level of theory using Gaussian 16 software.⁶ TheNCIplot⁷ isosurfaces correspond to both favorable and unfavorable interactions, as differentiated by the sign of the second density Hessian eigenvalue and defined by the isosurface color. The color scheme is a red–yellow–green–blue scale with red for repulsive (ρ_{cut}^+) and blue for attractive (ρ_{cut}^-) NCI interaction density. Yellow and green surfaces correspond to weak repulsive and weak attractive interactions,

¹ (a) A.D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652. (b) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627.

² S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

³ F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.

⁴ R. Ahlrichs, M. Bar, M. Haser, H. Horn, C. Kolmel, *Chem. Phys. Lett.*, 1989, **162**, 165–169.

⁵ AIMAll (Version 19.10.12), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2019 (aim.tkgristmill.com)

⁶ Gaussian 16, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

⁷ E. R. Johnson, S. Keinan, P. Mori-Sanchez, J. Contreras-Garcia, A. J. Cohen and W. Yang, *J. Am. Chem. Soc.*, 2010, **132**, 6498–6506.

respectively. Finally, solvent effects have been evaluated using the conductor-like screening model COSMO,⁸ which is a variant of the dielectric continuum solvation models.⁹ We have used water ($\epsilon = 78.4$) as solvent.

Obtention of the interaction energies

PDB structures

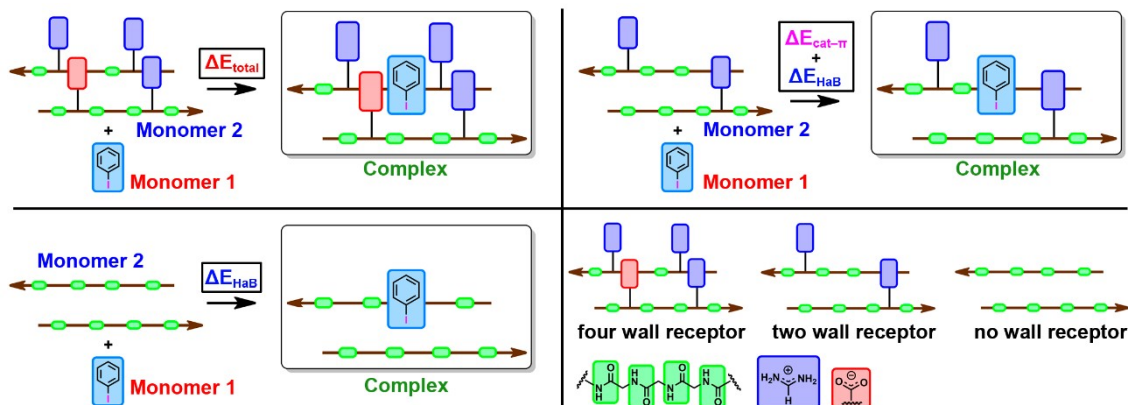


Figure S1. Schematic representation of the monomers and the complex used to compute the interaction energy values gathered in Table 1. $\Delta E_{\text{cation}-\pi}$ values were obtained as the difference between $(\Delta E_{\text{cat}-\pi} + \Delta E_{\text{HaB}}) - \Delta E_{\text{HaB}}$ values.

Complexes 5 to 14

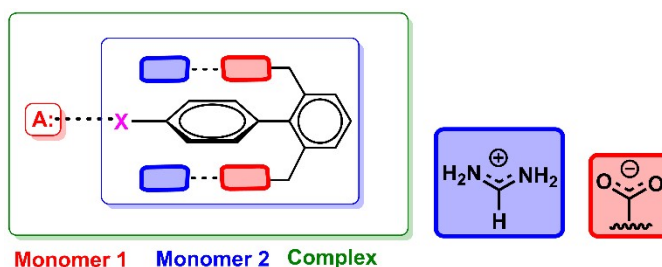


Figure S2. Schematic representation of the monomers and the complex used to compute the interaction energy values gathered in Table 2.

Additional MEP analysis

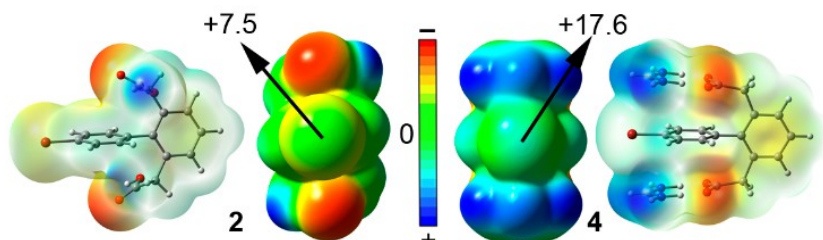


Figure S3. MEP (Molecular Electrostatic Potential) surface of compounds **2** and **4**. Energy values at concrete regions of the surface are given in kcal/mol (0.001 a.u.).

⁸ A. Klamt and G. Schüürmann, *J. Chem. Soc., Perkin Trans. 2*, 1993, 799–805.

⁹ A. Klampt, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2011, **1**, 699–709.

Cartesian coordinates of complexes 5 to 14

5.

C	-0.00000000	0.00000000	-3.04585589
C	-0.00000000	1.22034259	-3.75711655
C	-0.00000000	-1.22034259	-3.75711655
C	-0.00000000	1.19198433	-5.15364615
C	-0.00000000	-1.19198433	-5.15364615
C	-0.00000000	0.00000000	-5.85376032
H	-0.00000000	2.13165368	-5.69427180
H	-0.00000000	-2.13165368	-5.69427180
H	-0.00000000	0.00000000	-6.93699715
C	-0.00000000	-2.64090189	-3.18830160
H	0.88086765	-3.14421135	-3.59343279
H	-0.88086765	-3.14421135	-3.59343279
C	-0.00000000	0.00000000	-1.55030988
C	1.19751212	-0.00000000	-0.83895332
C	-1.19751212	0.00000000	-0.83895332
C	1.21059153	-0.00000000	0.54941358
H	2.13532727	-0.00000000	-1.37710960
C	-1.21059153	0.00000000	0.54941358
H	-2.13532727	0.00000000	-1.37710960
C	0.00000000	0.00000000	1.22702103
H	2.15022575	-0.00000000	1.08411336
H	-2.15022575	0.00000000	1.08411336
C	-0.00000000	-2.91754768	-1.68850849
O	-1.12206545	-3.05063712	-1.13023525
O	1.12206545	-3.05063712	-1.13023525
Br	0.00000000	0.00000000	3.35435003
C	0.00000000	2.64090189	-3.18830160
H	0.88086765	3.14421135	-3.59343279
H	-0.88086765	3.14421135	-3.59343279
C	0.00000000	2.91754768	-1.68850849
O	1.12206545	3.05063712	-1.13023525
O	-1.12206545	3.05063712	-1.13023525
C	-0.00000000	-3.46548228	2.06627763
N	1.14850733	-3.40435946	1.44339238
N	-1.14850733	-3.40435946	1.44339238
H	1.99157154	-3.42956698	1.99009803
H	-1.99157154	-3.42956698	1.99009803
H	1.17855546	-3.26325041	0.36280064
H	-1.17855546	-3.26325041	0.36280064
H	-0.00000000	-3.56587114	3.14795267
C	0.00000000	3.46548228	2.06627763
N	1.14850733	3.40435946	1.44339238
N	-1.14850733	3.40435946	1.44339238
H	1.99157154	3.42956698	1.99009803
H	-1.99157154	3.42956698	1.99009803
H	0.00000000	3.56587114	3.14795267
H	-1.17855546	3.26325041	0.36280064
H	1.17855546	3.26325041	0.36280064

N	0.00000000	0.00000000	6.15435024
C	0.00000000	0.00000000	7.35435030
H	0.00000000	0.00000000	8.18895035

6.

C	0.00000000	0.00000000	-3.05192336
C	0.00000000	1.22060579	-3.76258801
C	-0.00000000	-1.22060579	-3.76258801
C	0.00000000	1.19225049	-5.15911831
C	-0.00000000	-1.19225049	-5.15911831
C	0.00000000	-0.00000000	-5.85901325
H	0.00000000	2.13180535	-5.69996622
H	-0.00000000	-2.13180535	-5.69996622
H	0.00000000	0.00000000	-6.94225993
C	0.00000000	-2.64095429	-3.19233967
H	0.88083886	-3.14464133	-3.59710989
H	-0.88083886	-3.14464133	-3.59710989
C	0.00000000	-0.00000000	-1.55697145
C	1.19799838	-0.00000000	-0.84627599
C	-1.19799838	0.00000000	-0.84627599
C	1.21031549	-0.00000000	0.54144600
H	2.13521916	-0.00000000	-1.38519384
C	-1.21031549	0.00000000	0.54144600
H	-2.13521916	0.00000000	-1.38519384
C	0.00000000	0.00000000	1.21590165
H	2.14556605	-0.00000000	1.08364244
H	-2.14556605	0.00000000	1.08364244
C	0.00000000	-2.91644991	-1.69191866
O	-1.12195498	-3.04903672	-1.13322202
O	1.12195498	-3.04903672	-1.13322202
Br	0.00000000	0.00000000	3.14225909
C	0.00000000	2.64095429	-3.19233967
H	0.88083886	3.14464133	-3.59710989
H	-0.88083886	3.14464133	-3.59710989
C	0.00000000	2.91644991	-1.69191866
O	1.12195498	3.04903672	-1.13322202
O	-1.12195498	3.04903672	-1.13322202
C	0.00000000	-3.36561584	2.07546731
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N	-1.14825198	-3.33334414	1.45010637
H	1.99132434	-3.32801754	1.99726851
H	-1.99132434	-3.32801754	1.99726851
H	1.17807128	-3.22817623	0.36554719
H	-1.17807128	-3.22817623	0.36554719
H	0.00000000	-3.41646995	3.16055679
C	0.00000000	3.36561584	2.07546731
N	1.14825198	3.33334414	1.45010637
N	-1.14825198	3.33334414	1.45010637
H	1.99132434	3.32801754	1.99726851
H	-1.99132434	3.32801754	1.99726851
H	0.00000000	3.41646995	3.16055679

H	-1.17807128	3.22817623	0.36554719
H	1.17807128	3.22817623	0.36554719
O	0.00000000	0.00000000	7.85191001
C	0.00000000	0.00000000	6.72718377

7.

C	-0.00000000	0.00000000	-3.03308221
C	-0.00000000	1.22068239	-3.74355806
C	-0.00000000	-1.22068239	-3.74355806
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C	-0.00000000	-1.19230938	-5.14006466
C	-0.00000000	0.00000000	-5.83989481
H	-0.00000000	2.13183465	-5.68094722
H	-0.00000000	-2.13183465	-5.68094722
H	-0.00000000	0.00000000	-6.92312890
C	-0.00000000	-2.64094349	-3.17297802
H	0.88085756	-3.14469133	-3.57761665
H	-0.88085756	-3.14469133	-3.57761665
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C	-1.19808228	0.00000000	-0.82772865
C	1.21062709	-0.00000000	0.55999735
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C	-1.21062709	0.00000000	0.55999735
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C	0.00000000	-0.00000000	1.23341649
H	2.14570535	-0.00000000	1.10236858
H	-2.14570535	0.00000000	1.10236858
C	-0.00000000	-2.91602781	-1.67245472
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O	1.12194558	-3.04825402	-1.11363758
Br	0.00000000	-0.00000000	3.16001353
C	0.00000000	2.64094349	-3.17297802
H	0.88085756	3.14469133	-3.57761665
H	-0.88085756	3.14469133	-3.57761665
C	0.00000000	2.91602781	-1.67245472
O	1.12194558	3.04825402	-1.11363758
O	-1.12194558	3.04825402	-1.11363758
C	-0.00000000	-3.36727064	2.09492676
N	1.14825678	-3.33455994	1.46957231
N	-1.14825678	-3.33455994	1.46957231
H	1.99136364	-3.33034454	2.01670935
H	-1.99136364	-3.33034454	2.01670935
H	1.17805519	-3.22869773	0.38507493
H	-1.17805519	-3.22869773	0.38507493
H	-0.00000000	-3.41909485	3.17998613
C	0.00000000	3.36727064	2.09492676
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N	-1.14825678	3.33455994	1.46957231
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H	-1.99136364	3.33034454	2.01670935

H	0.00000000	3.41909485	3.17998613
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H	1.17805519	3.22869773	0.38507493
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O	0.00000000	-0.00000000	6.58442736

8.

C	0.00000000	0.00000000	-3.52908908
C	0.00000000	1.22220659	-4.23654073
C	-0.00000000	-1.22220659	-4.23654073
C	0.00000000	1.19364388	-5.63364285
C	-0.00000000	-1.19364388	-5.63364285
C	0.00000000	0.00000000	-6.33293127
H	0.00000000	2.13330205	-6.17519507
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H	0.00000000	0.00000000	-7.41679497
C	0.00000000	-2.64069169	-3.65780149
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H	-0.88062416	-3.14474473	-4.06405692
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C	-1.19829419	0.00000000	-1.33046522
C	1.20655239	-0.00000000	0.05527098
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H	-2.13479505	0.00000000	-1.87141046
C	0.00000000	0.00000000	0.74280293
H	2.14156826	-0.00000000	0.59934582
H	-2.14156826	0.00000000	0.59934582
C	0.00000000	-2.92965271	-2.15187028
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O	1.12215478	-3.07222092	-1.59853504
Br	0.00000000	0.00000000	2.65126027
C	0.00000000	2.64069169	-3.65780149
H	0.88062416	3.14474473	-4.06405692
H	-0.88062416	3.14474473	-4.06405692
C	0.00000000	2.92965271	-2.15187028
O	1.12215478	3.07222092	-1.59853504
O	-1.12215478	3.07222092	-1.59853504
C	0.00000000	-3.20120213	1.66868340
N	1.14823048	-3.24655013	1.04112715
N	-1.14823048	-3.24655013	1.04112715
H	1.98498714	-3.12221602	1.58425399
H	-1.98498714	-3.12221602	1.58425399
H	1.18080019	-3.20466333	-0.03136023
H	-1.18080019	-3.20466333	-0.03136023
H	0.00000000	-3.11660913	2.75062397
C	0.00000000	3.20120213	1.66868340
N	1.14823048	3.24655013	1.04112715
N	-1.14823048	3.24655013	1.04112715
H	1.98498714	3.12221602	1.58425399

H	-1.98498714	3.12221602	1.58425399
H	0.00000000	3.11660913	2.75062397
H	-1.18080019	3.20466333	-0.03136023
H	1.18080019	3.20466333	-0.03136023
O	0.00000000	0.00000000	5.40219808
N	0.00000000	0.00000000	6.66897004
O	0.00000000	1.08783078	7.28405789
O	-0.00000000	-1.08783078	7.28405789

9.

C	0.00000000	0.00000000	-3.07568131
C	0.00000000	1.22203649	-3.78376966
C	-0.00000000	-1.22203649	-3.78376966
C	0.00000000	1.19361799	-5.18105746
C	-0.00000000	-1.19361799	-5.18105746
C	0.00000000	0.00000000	-5.88058632
H	0.00000000	2.13341475	-5.72263310
H	-0.00000000	-2.13341475	-5.72263310
H	0.00000000	0.00000000	-6.96459877
C	-0.00000000	-2.64095419	-3.20535262
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H	-0.88055276	-3.14444822	-3.61283645
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C	1.19839309	-0.00000000	-0.87744965
C	-1.19839309	0.00000000	-0.87744965
C	1.20389379	-0.00000000	0.50854865
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C	0.00000000	0.00000000	1.20181030
H	2.14014755	-0.00000000	1.05249129
H	-2.14014755	0.00000000	1.05249129
C	0.00000000	-2.93670881	-1.69948851
O	-1.12221488	-3.08447602	-1.14790587
O	1.12221488	-3.08447602	-1.14790587
Br	0.00000000	0.00000000	3.13838964
C	0.00000000	2.64095419	-3.20535262
H	0.88055276	3.14444822	-3.61283645
H	-0.88055276	3.14444822	-3.61283645
C	0.00000000	2.93670881	-1.69948851
O	1.12221488	3.08447602	-1.14790587
O	-1.12221488	3.08447602	-1.14790587
C	0.00000000	-3.15279383	2.12648157
N	1.14841298	-3.22399043	1.50073492
N	-1.14841298	-3.22399043	1.50073492
H	1.98137894	-3.05421902	2.03746666
H	-1.98137894	-3.05421902	2.03746666
H	1.18032129	-3.19946123	0.42961234
H	-1.18032129	-3.19946123	0.42961234
H	0.00000000	-3.02420812	3.20392314
C	0.00000000	3.15279383	2.12648157

N	1.14841298	3.22399043	1.50073492
N	-1.14841298	3.22399043	1.50073492
H	1.98137894	3.05421902	2.03746666
H	-1.98137894	3.05421902	2.03746666
H	0.00000000	3.02420812	3.20392314
H	-1.18032129	3.19946123	0.42961234
H	1.18032129	3.19946123	0.42961234
Cl	0.00000000	0.00000000	6.09255853

10.

C	-0.00000000	-0.00000000	-3.31903808
C	-0.00000000	1.22023419	-4.03078283
C	-0.00000000	-1.22023419	-4.03078283
C	-0.00000000	1.19187159	-5.42741401
C	-0.00000000	-1.19187159	-5.42741401
C	-0.00000000	-0.00000000	-6.12768807
H	-0.00000000	2.13162385	-5.96798450
H	-0.00000000	-2.13162385	-5.96798450
H	-0.00000000	-0.00000000	-7.21097576
C	-0.00000000	-2.64137799	-3.46304089
H	0.88082356	-3.14405123	-3.86919592
H	-0.88082356	-3.14405123	-3.86919592
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C	-1.19716228	0.00000000	-1.11156872
C	1.20867559	-0.00000000	0.27661868
H	2.13506816	-0.00000000	-1.64977736
C	-1.20867559	0.00000000	0.27661868
H	-2.13506816	0.00000000	-1.64977736
C	0.00000000	0.00000000	0.96000523
H	2.14904626	-0.00000000	0.81069882
H	-2.14904626	0.00000000	0.81069882
C	-0.00000000	-2.92235461	-1.96363278
O	-1.12214128	-3.05830122	-1.40635954
O	1.12214128	-3.05830122	-1.40635954
I	0.00000000	0.00000000	3.08434248
C	0.00000000	2.64137799	-3.46304089
H	0.88082356	3.14405123	-3.86919592
H	-0.88082356	3.14405123	-3.86919592
C	0.00000000	2.92235461	-1.96363278
O	1.12214128	3.05830122	-1.40635954
O	-1.12214128	3.05830122	-1.40635954
C	0.00000000	-3.42538984	1.79761519
N	1.14850078	-3.38828585	1.17268364
N	-1.14850078	-3.38828585	1.17268364
H	1.99043954	-3.37796974	1.72156158
H	-1.99043954	-3.37796974	1.72156158
H	1.17859478	-3.26299283	0.09122667
H	-1.17859478	-3.26299283	0.09122667
H	0.00000000	-3.48488415	2.88205166
C	0.00000000	3.42538984	1.79761519

N	1.14850078	3.38828585	1.17268364
N	-1.14850078	3.38828585	1.17268364
H	1.99043954	3.37796974	1.72156158
H	-1.99043954	3.37796974	1.72156158
H	0.00000000	3.48488415	2.88205166
H	-1.17859478	3.26299283	0.09122667
H	1.17859478	3.26299283	0.09122667
N	0.00000000	0.00000000	6.55884921
C	0.00000000	0.00000000	7.70473433
H	0.00000000	0.00000000	8.77244738

11.

C	0.00000000	0.00000000	-3.32958385
C	0.00000000	1.22025039	-4.04113931
C	-0.00000000	-1.22025039	-4.04113931
C	0.00000000	1.19191218	-5.43769370
C	-0.00000000	-1.19191218	-5.43769370
C	0.00000000	0.00000000	-6.13787077
H	0.00000000	2.13160915	-5.97827726
H	-0.00000000	-2.13160915	-5.97827726
H	0.00000000	0.00000000	-7.22110384
C	0.00000000	-2.64101139	-3.47276136
H	0.88086206	-3.14414693	-3.87814759
H	-0.88086206	-3.14414693	-3.87814759
C	0.00000000	0.00000000	-1.83394494
C	1.19737458	-0.00000000	-1.12225110
C	-1.19737458	0.00000000	-1.12225110
C	1.20976549	-0.00000000	0.26603951
H	2.13521845	-0.00000000	-1.66044983
C	-1.20976549	0.00000000	0.26603951
H	-2.13521845	0.00000000	-1.66044983
C	0.00000000	0.00000000	0.94625816
H	2.14981546	-0.00000000	0.80031535
H	-2.14981546	0.00000000	0.80031535
C	0.00000000	-2.91865391	-1.97318596
O	-1.12208648	-3.05249452	-1.41511222
O	1.12208648	-3.05249452	-1.41511222
I	0.00000000	0.00000000	3.07220181
C	0.00000000	2.64101139	-3.47276136
H	0.88086206	3.14414693	-3.87814759
H	-0.88086206	3.14414693	-3.87814759
C	0.00000000	2.91865391	-1.97318596
O	1.12208648	3.05249452	-1.41511222
O	-1.12208648	3.05249452	-1.41511222
C	0.00000000	-3.45798025	1.78212161
N	1.14847838	-3.40020705	1.15890557
N	-1.14847838	-3.40020705	1.15890557
H	1.99140344	-3.42019755	1.70599521
H	-1.99140344	-3.42019755	1.70599521
H	1.17842989	-3.26191413	0.07776829
H	-1.17842989	-3.26191413	0.07776829

H	0.00000000	-3.55227495	2.86430590
C	0.00000000	3.45798025	1.78212161
N	1.14847838	3.40020705	1.15890557
N	-1.14847838	3.40020705	1.15890557
H	1.99140344	3.42019755	1.70599521
H	-1.99140344	3.42019755	1.70599521
H	0.00000000	3.55227495	2.86430590
H	-1.17842989	3.26191413	0.07776829
H	1.17842989	3.26191413	0.07776829
O	0.00000000	0.00000000	7.88705664
C	0.00000000	0.00000000	6.76253826

12.

C	-0.00000000	0.00000000	-3.31380283
C	-0.00000000	1.22032419	-4.02512408
C	-0.00000000	-1.22032419	-4.02512408
C	-0.00000000	1.19197158	-5.42166608
C	-0.00000000	-1.19197158	-5.42166608
C	-0.00000000	0.00000000	-6.12178801
H	-0.00000000	2.13164615	-5.96228081
H	-0.00000000	-2.13164615	-5.96228081
H	-0.00000000	0.00000000	-7.20501940
C	-0.00000000	-2.64096659	-3.45645504
H	0.88085456	-3.14417462	-3.86175697
H	-0.88085456	-3.14417462	-3.86175697
C	-0.00000000	0.00000000	-1.81829382
C	1.19746608	-0.00000000	-1.10682587
C	-1.19746608	0.00000000	-1.10682587
C	1.21016589	-0.00000000	0.28146633
H	2.13526745	-0.00000000	-1.64505741
C	-1.21016589	0.00000000	0.28146633
H	-2.13526745	0.00000000	-1.64505741
C	0.00000000	0.00000000	0.96040307
H	2.14999405	-0.00000000	0.81598806
H	-2.14999405	0.00000000	0.81598806
C	-0.00000000	-2.91849361	-1.95679293
O	-1.12206958	-3.05228162	-1.39867079
O	1.12206958	-3.05228162	-1.39867079
I	0.00000000	0.00000000	3.08649043
C	0.00000000	2.64096659	-3.45645504
H	0.88085456	3.14417462	-3.86175697
H	-0.88085456	3.14417462	-3.86175697
C	0.00000000	2.91849361	-1.95679293
O	1.12206958	3.05228162	-1.39867079
O	-1.12206958	3.05228162	-1.39867079
C	0.00000000	-3.45799785	1.79873703
N	1.14848778	-3.40180394	1.17536459
N	-1.14848778	-3.40180394	1.17536459
H	1.99142464	-3.42010975	1.72252503
H	-1.99142464	-3.42010975	1.72252503
H	1.17844688	-3.26380484	0.09426411

H	-1.17844688	-3.26380484	0.09426411
H	0.00000000	-3.55010705	2.88111281
C	0.00000000	3.45799785	1.79873703
N	1.14848778	3.40180394	1.17536459
N	-1.14848778	3.40180394	1.17536459
H	1.99142464	3.42010975	1.72252503
H	-1.99142464	3.42010975	1.72252503
H	0.00000000	3.55010705	2.88111281
H	-1.17844688	3.26380484	0.09426411
H	1.17844688	3.26380484	0.09426411
C	0.00000000	0.00000000	7.77665709
O	0.00000000	0.00000000	6.65118810

13.

C	0.00000000	0.00000000	-3.76595765
C	0.00000000	1.22077669	-4.47741740
C	-0.00000000	-1.22077669	-4.47741740
C	0.00000000	1.19231449	-5.87463482
C	-0.00000000	-1.19231449	-5.87463482
C	0.00000000	0.00000000	-6.57510304
H	0.00000000	2.13251275	-6.41525744
H	-0.00000000	-2.13251275	-6.41525744
H	0.00000000	0.00000000	-7.65896621
C	0.00000000	-2.64173839	-3.90701236
H	0.88070686	-3.14357012	-4.31573299
H	-0.88070686	-3.14357012	-4.31573299
C	0.00000000	0.00000000	-2.27267924
C	1.19669209	-0.00000000	-1.56099649
C	-1.19669209	0.00000000	-1.56099649
C	1.20357958	-0.00000000	-0.17383829
H	2.13465566	-0.00000000	-2.10002633
C	-1.20357958	0.00000000	-0.17383829
H	-2.13465566	0.00000000	-2.10002633
C	0.00000000	0.00000000	0.52514076
H	2.14499626	-0.00000000	0.36040715
H	-2.14499626	0.00000000	0.36040715
C	-0.00000000	-2.93724751	-2.40471115
O	-1.12253558	-3.08301062	-1.85298291
O	1.12253558	-3.08301062	-1.85298291
I	0.00000000	0.00000000	2.64513311
C	0.00000000	2.64173839	-3.90701236
H	0.88070686	3.14357012	-4.31573299
H	-0.88070686	3.14357012	-4.31573299
C	0.00000000	2.93724751	-2.40471115
O	1.12253558	3.08301062	-1.85298291
O	-1.12253558	3.08301062	-1.85298291
C	0.00000000	-3.31036804	1.39797142
N	1.14887428	-3.33059944	0.77065878
N	-1.14887428	-3.33059944	0.77065878
H	1.98489874	-3.22640983	1.31912691
H	-1.98489874	-3.22640983	1.31912691

H	1.18149968	-3.25023813	-0.30164950
H	-1.18149968	-3.25023813	-0.30164950
H	0.00000000	-3.27366643	2.48234440
C	0.00000000	3.31036804	1.39797142
N	1.14887428	3.33059944	0.77065878
N	-1.14887428	3.33059944	0.77065878
H	1.98489874	3.22640983	1.31912691
H	-1.98489874	3.22640983	1.31912691
H	0.00000000	3.27366643	2.48234440
H	-1.18149968	3.25023813	-0.30164950
H	1.18149968	3.25023813	-0.30164950
O	0.00000000	0.00000000	5.39559569
N	0.00000000	0.00000000	6.66666441
O	0.00000000	1.08725418	7.27686584
O	-0.00000000	-1.08725418	7.27686584

14.

C	0.00000000	0.00000000	-3.34945418
C	0.00000000	1.22011029	-4.06307013
C	-0.00000000	-1.22011029	-4.06307013
C	0.00000000	1.19180549	-5.46054251
C	-0.00000000	-1.19180549	-5.46054251
C	0.00000000	0.00000000	-6.16166300
H	0.00000000	2.13232745	-6.00087307
H	-0.00000000	-2.13232745	-6.00087307
H	0.00000000	0.00000000	-7.24567397
C	0.00000000	-2.64269359	-3.49629799
H	0.88066086	-3.14289543	-3.90746472
H	-0.88066086	-3.14289543	-3.90746472
C	0.00000000	0.00000000	-1.85572087
C	1.19650628	-0.00000000	-1.14280982
C	-1.19650628	0.00000000	-1.14280982
C	1.19948219	-0.00000000	0.24519458
H	2.13476076	-0.00000000	-1.68248736
C	-1.19948219	0.00000000	0.24519458
H	-2.13476076	0.00000000	-1.68248736
C	0.00000000	0.00000000	0.95256203
H	2.14304825	-0.00000000	0.77864022
H	-2.14304825	0.00000000	0.77864022
C	0.00000000	-2.94809561	-1.99558318
O	-1.12273888	-3.10043542	-1.44626574
O	1.12273888	-3.10043542	-1.44626574
I	0.00000000	0.00000000	3.12219199
C	0.00000000	2.64269359	-3.49629799
H	0.88066086	3.14289543	-3.90746472
H	-0.88066086	3.14289543	-3.90746472
C	0.00000000	2.94809561	-1.99558318
O	1.12273888	3.10043542	-1.44626574
O	-1.12273888	3.10043542	-1.44626574
C	0.00000000	-3.25955803	1.80929879
N	1.14932418	-3.30998304	1.18382675

N	-1.14932418	-3.30998304	1.18382675
H	1.98066854	-3.15301513	1.72698739
H	-1.98066854	-3.15301513	1.72698739
H	1.18118839	-3.24922743	0.11150427
H	-1.18118839	-3.24922743	0.11150427
H	0.00000000	-3.17143293	2.89024777
C	0.00000000	3.25955803	1.80929879
N	1.14932418	3.30998304	1.18382675
N	-1.14932418	3.30998304	1.18382675
H	1.98066854	3.15301513	1.72698739
H	-1.98066854	3.15301513	1.72698739
H	0.00000000	3.17143293	2.89024777
H	-1.18118839	3.24922743	0.11150427
H	1.18118839	3.24922743	0.11150427
Cl	0.00000000	0.00000000	6.05523942

Cartesian coordinates of PDB models

3D7H-four wall receptor

C	6.1016398	-1.3660303	4.3659165
C	5.8666398	-0.4480303	3.1739165
O	6.7646398	0.2949697	2.7549165
N	4.6326398	-0.4990303	2.6439165
C	4.2126398	0.4019697	1.5579165
C	2.8556398	0.9399697	2.0479165
O	2.0176398	0.1749697	2.4529165
C	4.0496398	-0.3770303	0.2289165
C	3.8026398	0.5049697	-1.0030835
C	3.6566398	-0.3260303	-2.2990835
N	3.4246398	0.4939697	-3.4750835
C	3.3626398	0.0349697	-4.7220835
N	3.5206398	-1.2770303	-4.9790835
N	3.1266398	0.8769697	-5.7130835
N	2.6906398	2.2529697	2.0459165
C	1.4056398	2.8449697	2.4719165
C	0.9846398	3.8949697	1.4449165
O	1.7736398	4.7349697	1.0609165
N	-0.3123602	3.8959697	1.0939165
C	-0.9123602	4.9839697	0.3029165
C	-2.1283602	5.3979697	1.1259165
O	-2.8723602	4.5409697	1.5809165
C	-1.5033602	4.4969697	-1.0200835
C	-0.4543602	4.1159697	-2.0570835
O	0.7776398	4.1429697	-1.7680835
O	-0.8663602	3.8019697	-3.2070835
N	-2.3143602	6.7039697	1.3539165
C	-3.4993602	7.1079697	2.1019165
C	-5.8573602	4.2089697	3.3399165
C	-5.6743602	2.7089697	3.0719165
O	-6.6353602	1.9029697	3.1049165
N	-4.4123602	2.3559697	2.7809165
C	-4.0593602	0.9529697	2.4899165
C	-2.5773602	0.8189697	2.8809165
O	-1.8323602	1.7959697	2.8549165
C	-4.2453602	0.6299697	0.9939165
C	-3.3763602	1.4119697	0.0659165
C	-3.8443602	1.2469697	-1.4280835
N	-3.9233602	-0.1670303	-1.8490835
C	-3.8413602	-0.5720303	-3.1120835
N	-3.9563602	-1.8930303	-3.3700835
N	-3.7063602	0.2969697	-4.0970835
N	-2.2033602	-0.4140303	3.2139165
C	-0.8193602	-0.6810303	3.6419165
C	-0.4973602	-2.1480303	3.3689165
O	-1.3533602	-3.0080303	3.5849165
N	0.7596398	-2.4450303	2.9689165
C	1.1516398	-3.8420303	2.7879165

C	2.6446398	-3.9170303	2.8689165
O	3.3076398	-2.8970303	2.8249165
C	0.7206398	-4.4240303	1.4279165
C	1.3476398	-3.7940303	0.2389165
C	0.9476398	-4.5280303	-1.0420835
N	-0.5253602	-4.5590303	-1.2260835
C	-1.1333602	-4.7780303	-2.3970835
N	-0.4283602	-4.9970303	-3.4950835
N	-2.4753602	-4.8110303	-2.4720835
N	3.1556398	-5.1370303	2.9279165
C	4.6266398	-5.3210303	2.7859165
I	0.1206398	0.0289697	-0.5190835
C	-0.0703602	-0.2600303	-2.6480835
C	0.0476398	0.7739697	-3.5790835
C	-0.0973602	0.5999697	-4.9750835
C	-0.3343602	-1.5150303	-3.2200835
C	-0.4493602	-1.6990303	-4.6190835
C	-0.3353602	-0.6660303	-5.5400835
H	5.4094971	-2.2216412	4.3905758
H	3.2246839	-1.0989025	0.3603664
H	4.9732489	-0.9626642	0.0870426
H	2.9038331	1.1299359	-0.8693998
H	4.6500733	1.2011704	-1.1291555
H	2.8149156	-1.0349254	-2.1771757
H	4.5808360	-0.9146451	-2.4447098
H	3.1363937	1.4587409	-3.3083130
H	3.8627237	-1.8855984	-4.2461687
H	3.6960652	-1.5833105	-5.9293227
H	2.9741039	1.8655425	-5.5372136
H	3.0242307	0.5653213	-6.6709926
H	4.9783760	1.1846924	1.4636242
H	0.6645828	2.0515043	2.6056251
H	-2.1581958	3.6361767	-0.8303831
H	-2.1439752	5.2807607	-1.4594316
H	-0.1530492	5.7583689	0.1443559
H	-4.4197895	6.8308298	1.5634135
H	-5.6407686	4.4196184	4.4003159
H	-5.1730402	4.8051844	2.7210456
H	-4.0720781	-0.4625735	0.8782878
H	-5.3148301	0.8061253	0.7831548
H	-3.4439599	2.4859305	0.2973183
H	-2.3191161	1.1433455	0.1528633
H	-4.8352945	1.7129665	-1.5613695
H	-3.1147182	1.7776498	-2.0654815
H	-4.1533573	-0.8420127	-1.1270954
H	-3.4870606	1.2711804	-3.8960624
H	-3.4632774	-0.0183695	-5.0297329
H	-4.3260067	-2.4914183	-2.6423847
H	-4.1835267	-2.1817631	-4.3152397
H	-4.7167625	0.3041345	3.0870815
H	-0.1343655	0.0025064	3.1294473

H	0.9214471	-5.5099916	1.4359509
H	-0.3812218	-4.3197056	1.4184634
H	2.4477905	-3.8354077	0.2944889
H	1.0784759	-2.7289219	0.1643246
H	1.3229535	-5.5661658	-1.0315494
H	1.3876476	-4.0032996	-1.9072236
H	-1.0950983	-4.3911775	-0.4012138
H	-3.0113886	-4.9231239	-1.6170419
H	-2.9200081	-5.1823452	-3.3048767
H	0.5833091	-4.9781474	-3.4853457
H	-0.8722340	-5.2391137	-4.3729637
H	0.6670740	-4.4391709	3.5776551
H	5.1413269	-5.1814877	3.7493700
H	0.1682996	1.8259167	-3.2541675
H	-0.0418429	1.5051090	-5.5866702
H	-0.4630927	-2.3767344	-2.5658638
H	-0.6498026	-2.7164418	-4.9701530
H	-3.5187521	6.6163143	3.0860873
H	-3.4881630	8.1966034	2.2465649
H	-6.9033839	4.4750141	3.1417391
H	5.0070907	-4.5696950	2.0819515
H	4.8291691	-6.3333212	2.4110393
H	7.1425581	-1.7152042	4.3376127
H	5.9720956	-0.7820081	5.2918705
H	1.5335774	3.3591612	3.4391730
H	-0.7014839	-0.5102847	4.7274444
H	-0.4414549	-0.8235711	-6.6156047
H	-1.6668284	7.3895089	0.9850776
H	-3.6861294	3.0610451	2.6417347
H	-2.8798088	-1.1501361	3.3936757
H	1.4502842	-1.7019703	2.8090306
H	2.5695819	-5.9396665	3.1235966
H	3.9624162	-1.1968530	2.9469784
H	3.3764808	2.9003860	1.6653092
H	-0.9688509	3.2716322	1.5621322

3D7H-two wall receptor

C	6.10163980	-1.36603030	4.36591650
C	5.86663980	-0.44803030	3.17391650
O	6.76463980	0.29496970	2.75491650
N	4.63263980	-0.49903030	2.64391650
C	4.21263980	0.40196970	1.55791650
C	2.85563980	0.93996970	2.04791650
O	2.01763980	0.17496970	2.45291650
C	4.04963980	-0.37703030	0.22891650
C	3.80263980	0.50496970	-1.00308350
C	3.65663980	-0.32603030	-2.29908350
N	3.42463980	0.49396970	-3.47508350
C	3.36263980	0.03496970	-4.72208350
N	3.52063980	-1.27703030	-4.97908350
N	3.12663980	0.87696970	-5.71308350

N	2.69063980	2.25296970	2.04591650
C	1.40563980	2.84496970	2.47191650
C	0.98463980	3.89496970	1.44491650
O	1.77363980	4.73496970	1.06091650
N	-0.31236020	3.89596970	1.09391650
C	-0.91236020	4.98396970	0.30291650
C	-2.12836020	5.39796970	1.12591650
O	-2.87236020	4.54096970	1.58091650
N	-2.31436020	6.70396970	1.35391650
C	-3.49936020	7.10796970	2.10191650
C	-5.85736020	4.20896970	3.33991650
C	-5.67436020	2.70896970	3.07191650
O	-6.63536020	1.90296970	3.10491650
N	-4.41236020	2.35596970	2.78091650
C	-4.05936020	0.95296970	2.48991650
C	-2.57736020	0.81896970	2.88091650
O	-1.83236020	1.79596970	2.85491650
C	-4.24536020	0.62996970	0.99391650
C	-3.37636020	1.41196970	0.06591650
C	-3.84436020	1.24696970	-1.42808350
N	-3.92336020	-0.16703030	-1.84908350
C	-3.84136020	-0.57203030	-3.11208350
N	-3.95636020	-1.89303030	-3.37008350
N	-3.70636020	0.29696970	-4.09708350
N	-2.20336020	-0.41403030	3.21391650
C	-0.81936020	-0.68103030	3.64191650
C	-0.49736020	-2.14803030	3.36891650
O	-1.35336020	-3.00803030	3.58491650
N	0.75963980	-2.44503030	2.96891650
C	1.15163980	-3.84203030	2.78791650
C	2.64463980	-3.91703030	2.86891650
O	3.30763980	-2.89703030	2.82491650
N	3.15563980	-5.13703030	2.92791650
C	4.62663980	-5.32103030	2.78591650
I	0.12063980	0.02896970	-0.51908350
C	-0.07036020	-0.26003030	-2.64808350
C	0.04763980	0.77396970	-3.57908350
C	-0.09736020	0.59996970	-4.97508350
C	-0.33436020	-1.51503030	-3.22008350
C	-0.44936020	-1.69903030	-4.61908350
C	-0.33536020	-0.66603030	-5.54008350
H	5.40949710	-2.22164120	4.39057580
H	3.22468390	-1.09890250	0.36036640
H	4.97324890	-0.96266420	0.08704260
H	2.90383310	1.12993590	-0.86939980
H	4.65007330	1.20117040	-1.12915550
H	2.81491560	-1.03492540	-2.17717570
H	4.58083600	-0.91464510	-2.44470980
H	3.13639370	1.45874090	-3.30831300
H	3.86272370	-1.88559840	-4.24616870
H	3.69606520	-1.58331050	-5.92932270

H	2.97410390	1.86554250	-5.53721360
H	3.02423070	0.56532130	-6.67099260
H	4.97837600	1.18469240	1.46362420
H	0.66458280	2.05150430	2.60562510
H	-0.15304920	5.75836890	0.14435590
H	-4.41978950	6.83082980	1.56341350
H	-5.64076860	4.41961840	4.40031590
H	-5.17304020	4.80518440	2.72104560
H	-4.07207810	-0.46257350	0.87828780
H	-5.31483010	0.80612530	0.78315480
H	-3.44395990	2.48593050	0.29731830
H	-2.31911610	1.14334550	0.15286330
H	-4.83529450	1.71296650	-1.56136950
H	-3.11471820	1.77764980	-2.06548150
H	-4.15335730	-0.84201270	-1.12709540
H	-3.48706060	1.27118040	-3.89606240
H	-3.46327740	-0.01836950	-5.02973290
H	-4.32600670	-2.49141830	-2.64238470
H	-4.18352670	-2.18176310	-4.31523970
H	-4.71676250	0.30413450	3.08708150
H	-0.13436550	0.00250640	3.12944730
H	0.66707400	-4.43917090	3.57765510
H	5.14132690	-5.18148770	3.74937000
H	0.16829960	1.82591670	-3.25416750
H	-0.04184290	1.50510900	-5.58667020
H	-0.46309270	-2.37673440	-2.56586380
H	-0.64980260	-2.71644180	-4.97015300
H	-3.51875210	6.61631430	3.08608730
H	-3.48816300	8.19660340	2.24656490
H	-6.90338390	4.47501410	3.14173910
H	5.00709070	-4.56969500	2.08195150
H	4.82916910	-6.33332120	2.41103930
H	7.14255810	-1.71520420	4.33761270
H	5.97209560	-0.78200810	5.29187050
H	1.53357740	3.35916120	3.43917300
H	-0.70148390	-0.51028470	4.72744440
H	-0.44145490	-0.82357110	-6.61560470
H	-1.66682840	7.38950890	0.98507760
H	-3.68612940	3.06104510	2.64173470
H	-2.87980880	-1.15013610	3.39367570
H	1.45028420	-1.70197030	2.80903060
H	2.56958190	-5.93966650	3.12359660
H	3.96241620	-1.19685300	2.94697840
H	3.37648080	2.90038600	1.66530920
H	-0.96885090	3.27163220	1.56213220
H	-1.32603821	4.64308782	-0.62313428
H	0.85233553	-4.24619523	1.84347611

3D7H-no wall receptor

C	6.10163980	-1.36603030	4.36591650
C	5.86663980	-0.44803030	3.17391650
O	6.76463980	0.29496970	2.75491650
N	4.63263980	-0.49903030	2.64391650
C	4.21263980	0.40196970	1.55791650
C	2.85563980	0.93996970	2.04791650
O	2.01763980	0.17496970	2.45291650
N	2.69063980	2.25296970	2.04591650
C	1.40563980	2.84496970	2.47191650
C	0.98463980	3.89496970	1.44491650
O	1.77363980	4.73496970	1.06091650
N	-0.31236020	3.89596970	1.09391650
C	-0.91236020	4.98396970	0.30291650
C	-2.12836020	5.39796970	1.12591650
O	-2.87236020	4.54096970	1.58091650
N	-2.31436020	6.70396970	1.35391650
C	-3.49936020	7.10796970	2.10191650
C	-5.85736020	4.20896970	3.33991650
C	-5.67436020	2.70896970	3.07191650
O	-6.63536020	1.90296970	3.10491650
N	-4.41236020	2.35596970	2.78091650
C	-4.05936020	0.95296970	2.48991650
C	-2.57736020	0.81896970	2.88091650
O	-1.83236020	1.79596970	2.85491650
N	-2.20336020	-0.41403030	3.21391650
C	-0.81936020	-0.68103030	3.64191650
C	-0.49736020	-2.14803030	3.36891650
O	-1.35336020	-3.00803030	3.58491650
N	0.75963980	-2.44503030	2.96891650
C	1.15163980	-3.84203030	2.78791650
C	2.64463980	-3.91703030	2.86891650
O	3.30763980	-2.89703030	2.82491650
N	3.15563980	-5.13703030	2.92791650
C	4.62663980	-5.32103030	2.78591650
I	0.12063980	0.02896970	-0.51908350
C	-0.07036020	-0.26003030	-2.64808350
C	0.04763980	0.77396970	-3.57908350
C	-0.09736020	0.59996970	-4.97508350
C	-0.33436020	-1.51503030	-3.22008350
C	-0.44936020	-1.69903030	-4.61908350
C	-0.33536020	-0.66603030	-5.54008350
H	5.40949710	-2.22164120	4.39057580
H	4.97837600	1.18469240	1.46362420
H	0.66458280	2.05150430	2.60562510
H	-0.15304920	5.75836890	0.14435590
H	-4.41978950	6.83082980	1.56341350
H	-5.64076860	4.41961840	4.40031590
H	-5.17304020	4.80518440	2.72104560
H	-4.71676250	0.30413450	3.08708150
H	-0.13436550	0.00250640	3.12944730

H	0.66707400	-4.43917090	3.57765510
H	5.14132690	-5.18148770	3.74937000
H	0.16829960	1.82591670	-3.25416750
H	-0.04184290	1.50510900	-5.58667020
H	-0.46309270	-2.37673440	-2.56586380
H	-0.64980260	-2.71644180	-4.97015300
H	-3.51875210	6.61631430	3.08608730
H	-3.48816300	8.19660340	2.24656490
H	-6.90338390	4.47501410	3.14173910
H	5.00709070	-4.56969500	2.08195150
H	4.82916910	-6.33332120	2.41103930
H	7.14255810	-1.71520420	4.33761270
H	5.97209560	-0.78200810	5.29187050
H	1.53357740	3.35916120	3.43917300
H	-0.70148390	-0.51028470	4.72744440
H	-0.44145490	-0.82357110	-6.61560470
H	-1.66682840	7.38950890	0.98507760
H	-3.68612940	3.06104510	2.64173470
H	-2.87980880	-1.15013610	3.39367570
H	1.45028420	-1.70197030	2.80903060
H	2.56958190	-5.93966650	3.12359660
H	3.96241620	-1.19685300	2.94697840
H	3.37648080	2.90038600	1.66530920
H	-0.96885090	3.27163220	1.56213220
H	-4.18844869	0.72879990	1.45165639
H	4.10005044	-0.13611073	0.63993333
H	-1.32603821	4.64308782	-0.62313428
H	0.85233553	-4.24619523	1.84347611

3IWW-four wall receptor

C	6.2707682	-1.2969273	4.3254271
C	6.0157682	-0.3589273	3.1684271
O	6.8957682	0.3440727	2.7524271
N	4.8107682	-0.4129273	2.6204271
C	4.3357682	0.4820727	1.5844271
C	2.9477682	0.9750727	2.0184271
O	2.1267682	0.1800727	2.4644271
C	4.1797682	-0.2969273	0.3054271
C	3.7477682	0.5160727	-0.8815729
C	3.6007682	-0.3989273	-2.1375729
N	3.3627682	0.4130727	-3.3355729
C	3.3887682	-0.0109273	-4.6075729
N	3.6937682	-1.2779273	-4.9325729
N	3.1217682	0.8660727	-5.5835729
N	2.7027682	2.2790727	1.9114271
C	1.4347682	2.9130727	2.3714271
C	0.9897682	3.9330727	1.3414271
O	1.8127682	4.7290727	0.8524271
N	-0.2802318	3.8600727	0.9764271
C	-0.9852318	4.9210727	0.2574271
C	-2.1942318	5.3430727	1.0824271

O	-3.0802318	4.5200727	1.4014271
C	-1.5842318	4.4060727	-1.0585729
C	-0.5562318	4.1950727	-2.1785729
O	0.6777682	4.2240727	-1.9385729
O	-1.0252318	3.9390727	-3.3365729
N	-2.3472318	6.6260727	1.3274271
C	-3.5512318	7.0420727	2.0204271
C	-5.8382318	4.0820727	3.3604271
C	-5.5912318	2.6080727	3.0694271
O	-6.5202318	1.7470727	3.0834271
N	-4.3402318	2.3160727	2.7544271
C	-3.9232318	0.9580727	2.5634271
C	-2.4322318	0.8200727	2.8834271
O	-1.6902318	1.8070727	2.8654271
C	-4.2352318	0.5450727	1.1184271
C	-3.3002318	1.1620727	0.0864271
C	-3.9162318	1.0670727	-1.3155729
N	-4.0022318	-0.3099273	-1.7865729
C	-4.0002318	-0.7029273	-3.0725729
N	-4.0722318	-1.9939273	-3.3565729
N	-3.8982318	0.1690727	-4.0595729
N	-2.0142318	-0.4009273	3.1904271
C	-0.6872318	-0.6619273	3.6594271
C	-0.3982318	-2.1369273	3.3964271
O	-1.2442318	-3.0119273	3.6264271
N	0.8027682	-2.3979273	2.9214271
C	1.2307682	-3.7709273	2.7204271
C	2.7337682	-3.8339273	2.7334271
O	3.3977682	-2.8029273	2.6984271
C	0.6687682	-4.2929273	1.3904271
C	1.2737682	-3.6339273	0.1894271
C	0.8447682	-4.3719273	-1.0745729
N	-0.6132318	-4.4389273	-1.1675729
C	-1.2982318	-4.6229273	-2.2865729
N	-2.6272318	-4.6969273	-2.2395729
N	-0.6802318	-4.7459273	-3.4445729
N	3.2767682	-5.0399273	2.8074271
C	4.7417682	-5.2449273	2.7224271
C	-0.3812318	-0.7849273	-5.5785729
C	-0.9432318	0.3940727	-5.0025729
C	-0.8462318	0.6660727	-3.5945729
C	-0.1832318	-0.1979273	-2.6895729
I	0.0157682	0.0870727	-0.4845729
C	0.3587682	-1.3489273	-3.3215729
C	0.2737682	-1.6569273	-4.7035729
H	5.4445617	-1.9938690	4.5336786
H	3.4594660	-1.1117437	0.5005904
H	5.1490710	-0.7810779	0.0946648
H	2.7996136	1.0472787	-0.7069139
H	4.5048133	1.2870259	-1.1075537
H	2.7702515	-1.1081806	-1.9845043

H	4.5345647	-0.9724542	-2.2717654
H	2.9820507	1.3460133	-3.1691734
H	4.0720522	-1.8908330	-4.2200846
H	3.9593742	-1.4966660	-5.8866434
H	2.8441919	1.8202881	-5.3696247
H	3.0831886	0.5873576	-6.5563175
H	5.0611827	1.3019466	1.4755876
H	0.6915313	2.1316894	2.5604119
H	-2.1043734	3.4569799	-0.8671114
H	-2.3495921	5.1056036	-1.4326867
H	-0.2641759	5.7248843	0.0596059
H	-4.4452076	6.7576169	1.4445207
H	-5.4984171	4.3198611	4.3821963
H	-5.2728130	4.7109278	2.6579809
H	-4.1958614	-0.5647932	1.0547345
H	-5.2862402	0.8288590	0.9501703
H	-3.1700651	2.2335741	0.3100957
H	-2.3214764	0.6929035	0.1046825
H	-4.9196690	1.5265139	-1.3210246
H	-3.2814411	1.6370596	-2.0155320
H	-4.3206856	-0.9863958	-1.0985910
H	-3.8607513	1.1675066	-3.8755692
H	-3.6118180	-0.1275872	-4.9844797
H	-4.0621930	-2.6854766	-2.6191567
H	-4.3959142	-2.2957428	-4.2682534
H	-4.5248664	0.3226544	3.2340626
H	0.0365165	-0.0067363	3.1625575
H	-0.4226149	-4.1371085	1.4680042
H	0.8267407	-5.3866512	1.3402835
H	2.3741465	-3.6678912	0.2286989
H	0.9903776	-2.5734753	0.1305550
H	1.2535151	-5.3983835	-1.0806205
H	1.2347558	-3.8484523	-1.9612917
H	-1.1182103	-4.4012282	-0.2857983
H	-3.0652144	-4.8592425	-1.3361088
H	-3.1101008	-5.1627199	-3.0034913
H	0.3265991	-4.6788594	-3.5127561
H	-1.1913250	-4.7986662	-4.3179349
H	0.8083667	-4.3867913	3.5324307
H	5.2454303	-4.3452507	3.0976022
H	-1.4065548	1.1634954	-5.6269862
H	-1.1873215	1.6756845	-3.2862141
H	0.9029846	-2.0603891	-2.6940370
H	0.7661787	-2.5614925	-5.0718872
H	-3.6203739	6.5628181	3.0090067
H	-3.5421166	8.1325958	2.1510962
H	-6.9140372	4.2850459	3.2918138
H	5.0252416	-6.1091706	3.3380308
H	5.0567103	-5.4227928	1.6810581
H	7.1916708	-1.8607919	4.1156001
H	6.4643481	-0.6941408	5.2266281

H	1.6230560	3.4400097	3.3222077
H	-0.5955665	-0.4845066	4.7482107
H	-1.6258206	7.2942407	1.0826349
H	-3.6560696	3.0587949	2.5890284
H	-0.8921088	3.2247800	1.4921718
H	-2.6893666	-1.1423279	3.3632020
H	3.3851073	2.9283611	1.5256136
H	4.1333128	-1.0959921	2.9433966
H	2.6845254	-5.8550981	2.9196886
H	1.4934449	-1.6471036	2.7829862
H	-0.4440202	-0.9753088	-6.6528627

3IWW-two wall receptor

C	6.27076820	-1.29692730	4.32542710
C	6.01576820	-0.35892730	3.16842710
O	6.89576820	0.34407270	2.75242710
N	4.81076820	-0.41292730	2.62042710
C	4.33576820	0.48207270	1.58442710
C	2.94776820	0.97507270	2.01842710
O	2.12676820	0.18007270	2.46442710
C	4.17976820	-0.29692730	0.30542710
C	3.74776820	0.51607270	-0.88157290
C	3.60076820	-0.39892730	-2.13757290
N	3.36276820	0.41307270	-3.33557290
C	3.38876820	-0.01092730	-4.60757290
N	3.69376820	-1.27792730	-4.93257290
N	3.12176820	0.86607270	-5.58357290
N	2.70276820	2.27907270	1.91142710
C	1.43476820	2.91307270	2.37142710
C	0.98976820	3.93307270	1.34142710
O	1.81276820	4.72907270	0.85242710
N	-0.28023180	3.86007270	0.97642710
C	-0.98523180	4.92107270	0.25742710
C	-2.19423180	5.34307270	1.08242710
O	-3.08023180	4.52007270	1.40142710
N	-2.34723180	6.62607270	1.32742710
C	-3.55123180	7.04207270	2.02042710
C	-5.83823180	4.08207270	3.36042710
C	-5.59123180	2.60807270	3.06942710
O	-6.52023180	1.74707270	3.08342710
N	-4.34023180	2.31607270	2.75442710
C	-3.92323180	0.95807270	2.56342710
C	-2.43223180	0.82007270	2.88342710
O	-1.69023180	1.80707270	2.86542710
C	-4.23523180	0.54507270	1.11842710
C	-3.30023180	1.16207270	0.08642710
C	-3.91623180	1.06707270	-1.31557290
N	-4.00223180	-0.30992730	-1.78657290
C	-4.00023180	-0.70292730	-3.07257290
N	-4.07223180	-1.99392730	-3.35657290
N	-3.89823180	0.16907270	-4.05957290

N	-2.01423180	-0.40092730	3.19042710
C	-0.68723180	-0.66192730	3.65942710
C	-0.39823180	-2.13692730	3.39642710
O	-1.24423180	-3.01192730	3.62642710
N	0.80276820	-2.39792730	2.92142710
C	1.23076820	-3.77092730	2.72042710
C	2.73376820	-3.83392730	2.73342710
O	3.39776820	-2.80292730	2.69842710
N	3.27676820	-5.03992730	2.80742710
C	4.74176820	-5.24492730	2.72242710
C	-0.38123180	-0.78492730	-5.57857290
C	-0.94323180	0.39407270	-5.00257290
C	-0.84623180	0.66607270	-3.59457290
C	-0.18323180	-0.19792730	-2.68957290
I	0.01576820	0.08707270	-0.48457290
C	0.35876820	-1.34892730	-3.32157290
C	0.27376820	-1.65692730	-4.70357290
H	5.44456170	-1.99386900	4.53367860
H	3.45946600	-1.11174370	0.50059040
H	5.14907100	-0.78107790	0.09466480
H	2.79961360	1.04727870	-0.70691390
H	4.50481330	1.28702590	-1.10755370
H	2.77025150	-1.10818060	-1.98450430
H	4.53456470	-0.97245420	-2.27176540
H	2.98205070	1.34601330	-3.16917340
H	4.07205220	-1.89083300	-4.22008460
H	3.95937420	-1.49666600	-5.88664340
H	2.84419190	1.82028810	-5.36962470
H	3.08318860	0.58735760	-6.55631750
H	5.06118270	1.30194660	1.47558760
H	0.69153130	2.13168940	2.56041190
H	-0.26417590	5.72488430	0.05960590
H	-4.44520760	6.75761690	1.44452070
H	-5.49841710	4.31986110	4.38219630
H	-5.27281300	4.71092780	2.65798090
H	-4.19586140	-0.56479320	1.05473450
H	-5.28624020	0.82885900	0.95017030
H	-3.17006510	2.23357410	0.31009570
H	-2.32147640	0.69290350	0.10468250
H	-4.91966900	1.52651390	-1.32102460
H	-3.28144110	1.63705960	-2.01553200
H	-4.32068560	-0.98639580	-1.09859100
H	-3.86075130	1.16750660	-3.87556920
H	-3.61181800	-0.12758720	-4.98447970
H	-4.06219300	-2.68547660	-2.61915670
H	-4.39591420	-2.29574280	-4.26825340
H	-4.52486640	0.32265440	3.23406260
H	0.03651650	-0.00673630	3.16255750
H	0.80836670	-4.38679130	3.53243070
H	5.24543030	-4.34525070	3.09760220
H	-1.40655480	1.16349540	-5.62698620

H	-1.18732150	1.67568450	-3.28621410
H	0.90298460	-2.06038910	-2.69403700
H	0.76617870	-2.56149250	-5.07188720
H	-3.62037390	6.56281810	3.00900670
H	-3.54211660	8.13259580	2.15109620
H	-6.91403720	4.28504590	3.29181380
H	5.02524160	-6.10917060	3.33803080
H	5.05671030	-5.42279280	1.68105810
H	7.19167080	-1.86079190	4.11560010
H	6.46434810	-0.69414080	5.22662810
H	1.62305600	3.44000970	3.32220770
H	-0.59556650	-0.48450660	4.74821070
H	-1.62582060	7.29424070	1.08263490
H	-3.65606960	3.05879490	2.58902840
H	-0.89210880	3.22478000	1.49217180
H	-2.68936660	-1.14232790	3.36320200
H	3.38510730	2.92836110	1.52561360
H	4.13331280	-1.09599210	2.94339660
H	2.68452540	-5.85509810	2.91968860
H	1.49344490	-1.64710360	2.78298620
H	-0.44402020	-0.97530880	-6.65286270
H	-1.40280617	4.56205634	-0.65998170
H	0.83909911	-4.13471959	1.79352338

3IWW-no wall receptor

C	6.27076820	-1.29692730	4.32542710
C	6.01576820	-0.35892730	3.16842710
O	6.89576820	0.34407270	2.75242710
N	4.81076820	-0.41292730	2.62042710
C	4.33576820	0.48207270	1.58442710
C	2.94776820	0.97507270	2.01842710
O	2.12676820	0.18007270	2.46442710
N	2.70276820	2.27907270	1.91142710
C	1.43476820	2.91307270	2.37142710
C	0.98976820	3.93307270	1.34142710
O	1.81276820	4.72907270	0.85242710
N	-0.28023180	3.86007270	0.97642710
C	-0.98523180	4.92107270	0.25742710
C	-2.19423180	5.34307270	1.08242710
O	-3.08023180	4.52007270	1.40142710
N	-2.34723180	6.62607270	1.32742710
C	-3.55123180	7.04207270	2.02042710
C	-5.83823180	4.08207270	3.36042710
C	-5.59123180	2.60807270	3.06942710
O	-6.52023180	1.74707270	3.08342710
N	-4.34023180	2.31607270	2.75442710
C	-3.92323180	0.95807270	2.56342710
C	-2.43223180	0.82007270	2.88342710
O	-1.69023180	1.80707270	2.86542710
N	-2.01423180	-0.40092730	3.19042710
C	-0.68723180	-0.66192730	3.65942710

C	-0.39823180	-2.13692730	3.39642710
O	-1.24423180	-3.01192730	3.62642710
N	0.80276820	-2.39792730	2.92142710
C	1.23076820	-3.77092730	2.72042710
C	2.73376820	-3.83392730	2.73342710
O	3.39776820	-2.80292730	2.69842710
N	3.27676820	-5.03992730	2.80742710
C	4.74176820	-5.24492730	2.72242710
C	-0.38123180	-0.78492730	-5.57857290
C	-0.94323180	0.39407270	-5.00257290
C	-0.84623180	0.66607270	-3.59457290
C	-0.18323180	-0.19792730	-2.68957290
I	0.01576820	0.08707270	-0.48457290
C	0.35876820	-1.34892730	-3.32157290
C	0.27376820	-1.65692730	-4.70357290
H	5.44456170	-1.99386900	4.53367860
H	5.06118270	1.30194660	1.47558760
H	0.69153130	2.13168940	2.56041190
H	-0.26417590	5.72488430	0.05960590
H	-4.44520760	6.75761690	1.44452070
H	-5.49841710	4.31986110	4.38219630
H	-5.27281300	4.71092780	2.65798090
H	-4.52486640	0.32265440	3.23406260
H	0.03651650	-0.00673630	3.16255750
H	0.80836670	-4.38679130	3.53243070
H	5.24543030	-4.34525070	3.09760220
H	-1.40655480	1.16349540	-5.62698620
H	-1.18732150	1.67568450	-3.28621410
H	0.90298460	-2.06038910	-2.69403700
H	0.76617870	-2.56149250	-5.07188720
H	-3.62037390	6.56281810	3.00900670
H	-3.54211660	8.13259580	2.15109620
H	-6.91403720	4.28504590	3.29181380
H	5.02524160	-6.10917060	3.33803080
H	5.05671030	-5.42279280	1.68105810
H	7.19167080	-1.86079190	4.11560010
H	6.46434810	-0.69414080	5.22662810
H	1.62305600	3.44000970	3.32220770
H	-0.59556650	-0.48450660	4.74821070
H	-1.62582060	7.29424070	1.08263490
H	-3.65606960	3.05879490	2.58902840
H	-0.89210880	3.22478000	1.49217180
H	-2.68936660	-1.14232790	3.36320200
H	3.38510730	2.92836110	1.52561360
H	4.13331280	-1.09599210	2.94339660
H	2.68452540	-5.85509810	2.91968860
H	1.49344490	-1.64710360	2.78298620
H	-0.44402020	-0.97530880	-6.65286270
H	-1.40280617	4.56205634	-0.65998170
H	-4.14073039	0.67016591	1.55610191
H	0.83909911	-4.13471959	1.79352338

H	4.22490666	-0.07152433	0.67550463
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4OC0-four wall receptor

C	5.1481945	-5.6157913	0.9809595
C	4.4002935	-4.7384933	1.9709695
O	4.5620845	-4.8980573	3.1875095
N	3.6025185	-3.8233303	1.4378685
C	2.7003035	-2.9859883	2.2218465
C	1.3494225	-3.0948063	1.5279595
O	1.2446305	-2.9049033	0.3078575
C	3.2472705	-1.5321343	2.2212355
C	2.3468615	-0.5067743	2.9757985
C	3.0165615	0.8896817	2.9819835
N	2.2642905	1.8585527	3.8010715
C	2.5956325	3.1480147	3.9944765
N	3.6899335	3.6761597	3.4370335
N	1.8221775	3.9323337	4.7589525
N	0.3022625	-3.3829333	2.2998115
C	-1.0672635	-3.4869123	1.7333845
C	-2.0333835	-2.6748083	2.6113425
O	-1.9995195	-2.7668673	3.8378155
N	-2.9057045	-1.9180503	1.9662735
C	-4.0708445	-1.3320823	2.6273585
C	-5.2911405	-1.7831063	1.8338375
O	-5.3207415	-1.6137533	0.6331795
C	-4.1090705	0.2059387	2.5398085
C	-2.9638795	0.9024367	3.2770605
O	-2.0088135	0.2582977	3.7329615
O	-3.0325625	2.1586837	3.3521005
N	-6.3463605	-2.2226433	2.5006945
C	-7.5035595	-2.6763343	1.7558735
C	-7.3095155	-2.1950693	-2.1528775
C	-6.1078165	-1.5934053	-2.8694635
O	-6.2286545	-1.0757733	-3.9976855
N	-4.9610625	-1.7104653	-2.2291455
C	-3.6884655	-1.2645933	-2.8582785
C	-2.5321145	-2.0108643	-2.2231745
O	-2.6493085	-2.5169033	-1.1047285
C	-3.4782975	0.2559877	-2.6640075
C	-3.3669155	0.7102837	-1.1505915
C	-3.6431925	2.2954957	-0.9753895
N	-2.6824625	3.0620437	-1.7578055
C	-2.2242095	4.2754327	-1.4373065
N	-1.3543595	4.8673817	-2.2582345
N	-2.6358345	4.8806367	-0.3130385
N	-1.4266735	-2.1086663	-2.9677305
C	-0.2955605	-2.8651933	-2.4849635
C	0.9358365	-2.3064663	-3.1664445
O	0.9016945	-2.0222273	-4.3795275
N	2.0346925	-2.2330733	-2.4236605
C	3.3031705	-1.7871493	-3.0197325

C	4.4473685	-2.3178373	-2.1904235
O	4.2155665	-2.8035913	-1.0857475
C	3.3593735	-0.2355023	-3.0689195
C	3.5275225	0.4098947	-1.7150935
C	3.7068305	1.9255897	-1.8585585
N	2.6645055	2.5084687	-2.7198715
C	2.5077555	3.8165607	-2.9358555
N	3.3046645	4.7059437	-2.3256725
N	1.5594885	4.2356817	-3.7682485
N	5.6750185	-2.2293443	-2.7059895
C	6.8687225	-2.5150743	-1.9037495
C	0.6371835	5.3121807	1.7025805
C	-0.2851355	4.4573527	2.3508465
C	-0.4434475	3.1034547	1.9580295
C	0.2747995	2.5281157	0.8966945
I	-0.0134505	0.4253897	0.2972915
C	1.1823745	3.3877577	0.2472175
C	1.3611665	4.7499237	0.6316555
H	5.1816318	-5.1986745	-0.0376937
H	3.3685485	-1.2248614	1.1682289
H	4.2479173	-1.5674276	2.6799396
H	1.3388141	-0.4479719	2.5479044
H	2.2274985	-0.8376026	4.0222197
H	3.0795619	1.2694986	1.9439081
H	4.0407906	0.8011659	3.3846736
H	1.3352321	1.5632067	4.1074882
H	4.3638591	3.0691140	2.9870988
H	4.0436473	4.5674382	3.7649642
H	0.9572087	3.5796021	5.1574278
H	1.9998043	4.9242847	4.8521100
H	2.6764926	-3.3869012	3.2456105
H	-1.0529560	-3.1572264	0.6904997
H	-4.0761756	0.5053160	1.4830550
H	-5.0652438	0.5808724	2.9391146
H	-4.0568399	-1.6577259	3.6751847
H	-7.9530140	-1.8456413	1.1903441
H	-7.3880081	-3.2607635	-2.4244879
H	-7.2096750	-2.1198361	-1.0613570
H	-2.5669626	0.5518316	-3.2227333
H	-4.3419880	0.7465130	-3.1433094
H	-4.1389881	0.1889462	-0.5667664
H	-2.3968092	0.4655589	-0.7211592
H	-4.6720253	2.5378227	-1.2866012
H	-3.5229056	2.5152816	0.0982893
H	-2.4652121	2.6909762	-2.6775711
H	-3.1898744	4.3633830	0.3654811
H	-2.1072598	5.6603807	0.0637004
H	-1.2015553	4.4784925	-3.1790629
H	-1.1831851	5.8621049	-2.1658302
H	-3.7668875	-1.4638677	-3.9382124
H	-0.2330282	-2.8063915	-1.3931021

H	4.1862647	0.0697544	-3.7360365
H	2.4260712	0.0584298	-3.5796749
H	4.4211879	0.0283036	-1.1982064
H	2.6644055	0.1860224	-1.0694629
H	4.6890118	2.1463743	-2.3135998
H	3.6696858	2.4035877	-0.8643788
H	1.9802743	1.8676760	-3.1122819
H	1.1920988	3.5832251	-4.4552866
H	1.5402860	5.2079965	-4.0595258
H	4.0140150	4.4075288	-1.6678906
H	3.2937775	5.6880406	-2.5761445
H	3.3418503	-2.1612890	-4.0555692
H	6.5602947	-2.6275782	-0.8572732
H	-0.9152560	4.8093300	3.1734038
H	-1.2179863	2.5431465	2.5301156
H	1.7521636	3.0072805	-0.5943914
H	2.0849504	5.3527135	0.0760254
H	-4.9212526	-2.0097728	-1.2529994
H	-1.4145697	-1.8519130	-3.9508833
H	2.0267064	-2.5167841	-1.4342167
H	5.7944072	-1.9292183	-3.6673232
H	3.5854826	-3.6753142	0.4332029
H	0.3721144	-3.4730864	3.3106352
H	-2.9594301	-1.9717058	0.9482192
H	-6.2730282	-2.4164189	3.4926002
H	7.3524386	-3.4509198	-2.2258996
H	7.5943746	-1.6922927	-1.9957965
H	-8.2187803	-1.6866469	-2.4982229
H	-8.2551118	-3.0724044	2.4517728
H	-7.2293740	-3.4650781	1.0376045
H	4.6530274	-6.5997546	0.9422184
H	6.1667486	-5.7784613	1.3593810
H	0.7701419	6.3555286	1.9995470
H	-1.3949443	-4.5394065	1.7582122
H	-0.3758497	-3.9358657	-2.7513306

4OC0-two wall receptor

C	5.14819450	-5.61579130	0.98095950
C	4.40029350	-4.73849330	1.97096950
O	4.56208450	-4.89805730	3.18750950
N	3.60251850	-3.82333030	1.43786850
C	2.70030350	-2.98598830	2.22184650
C	1.34942250	-3.09480630	1.52795950
O	1.24463050	-2.90490330	0.30785750
C	3.24727050	-1.53213430	2.22123550
C	2.34686150	-0.50677430	2.97579850
C	3.01656150	0.88968170	2.98198350
N	2.26429050	1.85855270	3.80107150
C	2.59563250	3.14801470	3.99447650
N	3.68993350	3.67615970	3.43703350
N	1.82217750	3.93233370	4.75895250

N	0.30226250	-3.38293330	2.29981150
C	-1.06726350	-3.48691230	1.73338450
C	-2.03338350	-2.67480830	2.61134250
O	-1.99951950	-2.76686730	3.83781550
N	-2.90570450	-1.91805030	1.96627350
C	-4.07084450	-1.33208230	2.62735850
C	-5.29114050	-1.78310630	1.83383750
O	-5.32074150	-1.61375330	0.63317950
N	-6.34636050	-2.22264330	2.50069450
C	-7.50355950	-2.67633430	1.75587350
C	-7.30951550	-2.19506930	-2.15287750
C	-6.10781650	-1.59340530	-2.86946350
O	-6.22865450	-1.07577330	-3.99768550
N	-4.96106250	-1.71046530	-2.22914550
C	-3.68846550	-1.26459330	-2.85827850
C	-2.53211450	-2.01086430	-2.22317450
O	-2.64930850	-2.51690330	-1.10472850
C	-3.47829750	0.25598770	-2.66400750
C	-3.36691550	0.71028370	-1.15059150
C	-3.64319250	2.29549570	-0.97538950
N	-2.68246250	3.06204370	-1.75780550
C	-2.22420950	4.27543270	-1.43730650
N	-1.35435950	4.86738170	-2.25823450
N	-2.63583450	4.88063670	-0.31303850
N	-1.42667350	-2.10866630	-2.96773050
C	-0.29556050	-2.86519330	-2.48496350
C	0.93583650	-2.30646630	-3.16644450
O	0.90169450	-2.02222730	-4.37952750
N	2.03469250	-2.23307330	-2.42366050
C	3.30317050	-1.78714930	-3.01973250
C	4.44736850	-2.31783730	-2.19042350
O	4.21556650	-2.80359130	-1.08574750
N	5.67501850	-2.22934430	-2.70598950
C	6.86872250	-2.51507430	-1.90374950
C	0.63718350	5.31218070	1.70258050
C	-0.28513550	4.45735270	2.35084650
C	-0.44344750	3.10345470	1.95802950
C	0.27479950	2.52811570	0.89669450
I	-0.01345050	0.42538970	0.29729150
C	1.18237450	3.38775770	0.24721750
C	1.36116650	4.74992370	0.63165550
H	5.18163180	-5.19867450	-0.03769370
H	3.36854850	-1.22486140	1.16822890
H	4.24791730	-1.56742760	2.67993960
H	1.33881410	-0.44797190	2.54790440
H	2.22749850	-0.83760260	4.02221970
H	3.07956190	1.26949860	1.94390810
H	4.04079060	0.80116590	3.38467360
H	1.33523210	1.56320670	4.10748820
H	4.36385910	3.06911400	2.98709880
H	4.04364730	4.56743820	3.76496420

H	0.95720870	3.57960210	5.15742780
H	1.99980430	4.92428470	4.85211000
H	2.67649260	-3.38690120	3.24561050
H	-1.05295600	-3.15722640	0.69049970
H	-4.05683990	-1.65772590	3.67518470
H	-7.95301400	-1.84564130	1.19034410
H	-7.38800810	-3.26076350	-2.42448790
H	-7.20967500	-2.11983610	-1.06135700
H	-2.56696260	0.55183160	-3.22273330
H	-4.34198800	0.74651300	-3.14330940
H	-4.13898810	0.18894620	-0.56676640
H	-2.39680920	0.46555890	-0.72115920
H	-4.67202530	2.53782270	-1.28660120
H	-3.52290560	2.51528160	0.09828930
H	-2.46521210	2.69097620	-2.67757110
H	-3.18987440	4.36338300	0.36548110
H	-2.10725980	5.66038070	0.06370040
H	-1.20155530	4.47849250	-3.17906290
H	-1.18318510	5.86210490	-2.16583020
H	-3.76688750	-1.46386770	-3.93821240
H	-0.23302820	-2.80639150	-1.39310210
H	3.34185030	-2.16128900	-4.05556920
H	6.56029470	-2.62757820	-0.85727320
H	-0.91525600	4.80933000	3.17340380
H	-1.21798630	2.54314650	2.53011560
H	1.75216360	3.00728050	-0.59439140
H	2.08495040	5.35271350	0.07602540
H	-4.92125260	-2.00977280	-1.25299940
H	-1.41456970	-1.85191300	-3.95088330
H	2.02670640	-2.51678410	-1.43421670
H	5.79440720	-1.92921830	-3.66732320
H	3.58548260	-3.67531420	0.43320290
H	0.37211440	-3.47308640	3.31063520
H	-2.95943010	-1.97170580	0.94821920
H	-6.27302820	-2.41641890	3.49260020
H	7.35243860	-3.45091980	-2.22589960
H	7.59437460	-1.69229270	-1.99579650
H	-8.21878030	-1.68664690	-2.49822290
H	-8.25511180	-3.07240440	2.45177280
H	-7.22937400	-3.46507810	1.03760450
H	4.65302740	-6.59975460	0.94221840
H	6.16674860	-5.77846130	1.35938100
H	0.77014190	6.35552860	1.99954700
H	-1.39494430	-4.53940650	1.75821220
H	-0.37584970	-3.93586570	-2.75133060
H	-4.09738715	-0.26414040	2.56656719
H	3.34188270	-0.71838668	-3.05361213

4OC0-no wall receptor

C	5.14819450	-5.61579130	0.98095950
C	4.40029350	-4.73849330	1.97096950

O	4.56208450	-4.89805730	3.18750950
N	3.60251850	-3.82333030	1.43786850
C	2.70030350	-2.98598830	2.22184650
C	1.34942250	-3.09480630	1.52795950
O	1.24463050	-2.90490330	0.30785750
N	0.30226250	-3.38293330	2.29981150
C	-1.06726350	-3.48691230	1.73338450
C	-2.03338350	-2.67480830	2.61134250
O	-1.99951950	-2.76686730	3.83781550
N	-2.90570450	-1.91805030	1.96627350
C	-4.07084450	-1.33208230	2.62735850
C	-5.29114050	-1.78310630	1.83383750
O	-5.32074150	-1.61375330	0.63317950
N	-6.34636050	-2.22264330	2.50069450
C	-7.50355950	-2.67633430	1.75587350
C	-7.30951550	-2.19506930	-2.15287750
C	-6.10781650	-1.59340530	-2.86946350
O	-6.22865450	-1.07577330	-3.99768550
N	-4.96106250	-1.71046530	-2.22914550
C	-3.68846550	-1.26459330	-2.85827850
C	-2.53211450	-2.01086430	-2.22317450
O	-2.64930850	-2.51690330	-1.10472850
N	-1.42667350	-2.10866630	-2.96773050
C	-0.29556050	-2.86519330	-2.48496350
C	0.93583650	-2.30646630	-3.16644450
O	0.90169450	-2.02222730	-4.37952750
N	2.03469250	-2.23307330	-2.42366050
C	3.30317050	-1.78714930	-3.01973250
C	4.44736850	-2.31783730	-2.19042350
O	4.21556650	-2.80359130	-1.08574750
N	5.67501850	-2.22934430	-2.70598950
C	6.86872250	-2.51507430	-1.90374950
C	0.63718350	5.31218070	1.70258050
C	-0.28513550	4.45735270	2.35084650
C	-0.44344750	3.10345470	1.95802950
C	0.27479950	2.52811570	0.89669450
I	-0.01345050	0.42538970	0.29729150
C	1.18237450	3.38775770	0.24721750
C	1.36116650	4.74992370	0.63165550
H	5.18163180	-5.19867450	-0.03769370
H	2.67649260	-3.38690120	3.24561050
H	-1.05295600	-3.15722640	0.69049970
H	-4.05683990	-1.65772590	3.67518470
H	-7.95301400	-1.84564130	1.19034410
H	-7.38800810	-3.26076350	-2.42448790
H	-7.20967500	-2.11983610	-1.06135700
H	-3.76688750	-1.46386770	-3.93821240
H	-0.23302820	-2.80639150	-1.39310210
H	3.34185030	-2.16128900	-4.05556920
H	6.56029470	-2.62757820	-0.85727320
H	-0.91525600	4.80933000	3.17340380

H	-1.21798630	2.54314650	2.53011560
H	1.75216360	3.00728050	-0.59439140
H	2.08495040	5.35271350	0.07602540
H	-4.92125260	-2.00977280	-1.25299940
H	-1.41456970	-1.85191300	-3.95088330
H	2.02670640	-2.51678410	-1.43421670
H	5.79440720	-1.92921830	-3.66732320
H	3.58548260	-3.67531420	0.43320290
H	0.37211440	-3.47308640	3.31063520
H	-2.95943010	-1.97170580	0.94821920
H	-6.27302820	-2.41641890	3.49260020
H	7.35243860	-3.45091980	-2.22589960
H	7.59437460	-1.69229270	-1.99579650
H	-8.21878030	-1.68664690	-2.49822290
H	-8.25511180	-3.07240440	2.45177280
H	-7.22937400	-3.46507810	1.03760450
H	4.65302740	-6.59975460	0.94221840
H	6.16674860	-5.77846130	1.35938100
H	0.77014190	6.35552860	1.99954700
H	-1.39494430	-4.53940650	1.75821220
H	-0.37584970	-3.93586570	-2.75133060
H	-4.09738715	-0.26414040	2.56656719
H	-3.54312683	-0.21305728	-2.72393317
H	3.34188270	-0.71838668	-3.05361213
H	3.07707532	-1.98451797	2.22142562

4OC1-four wall receptor

C	6.1371822	-1.3396734	4.3862626
C	5.8991822	-0.4406734	3.1812626
O	6.7931822	0.2943266	2.7822626
N	4.6761822	-0.4786734	2.6302626
C	4.2961822	0.4553266	1.5682626
C	2.9271822	0.9653266	2.0442626
O	2.1031822	0.1773266	2.5172626
C	4.1731822	-0.3186734	0.2382626
C	3.7741822	0.5153266	-0.9927374
C	3.6511822	-0.3566734	-2.2217374
N	3.3211822	0.4433266	-3.4047374
C	3.2871822	-0.0096734	-4.6557374
N	3.6211822	-1.2796734	-4.9407374
N	2.9551822	0.8323266	-5.6477374
N	2.7081822	2.2753266	1.9672626
C	1.4271822	2.8573266	2.4082626
C	0.9651822	3.8903266	1.3832626
O	1.7571822	4.7033266	0.9172626
N	-0.3288178	3.8803266	1.0692626
C	-0.9728178	4.9693266	0.3032626
C	-2.1618178	5.3813266	1.1292626
O	-2.9398178	4.5403266	1.5272626
C	-1.5438178	4.4913266	-1.0407374
C	-0.4788178	4.1563266	-2.0887374

O	0.7251822	4.1813266	-1.7897374
O	-0.8938178	3.8233266	-3.2367374
N	-2.3298178	6.6763266	1.3922626
C	-3.4938178	7.0973266	2.1652626
C	-5.8278178	4.1973266	3.4022626
C	-5.6188178	2.7183266	3.1042626
O	-6.5658178	1.9073266	3.1542626
N	-4.3728178	2.3653266	2.8212626
C	-4.0258178	0.9733266	2.5332626
C	-2.5298178	0.8223266	2.9282626
O	-1.7728178	1.7973266	2.9102626
C	-4.2888178	0.6323266	1.0652626
C	-3.4868178	1.4343266	0.0592626
C	-4.0358178	1.2723266	-1.4107374
N	-4.0388178	-0.1256734	-1.8477374
C	-3.9108178	-0.5496734	-3.1107374
N	-3.7998178	0.3183266	-4.1117374
N	-3.9638178	-1.8666734	-3.3617374
N	-2.1438178	-0.3996734	3.2892626
C	-0.7398178	-0.6676734	3.7032626
C	-0.4398178	-2.1446734	3.4472626
O	-1.3178178	-2.9916734	3.6412626
N	0.7661822	-2.4516734	2.9602626
C	1.1761822	-3.8446734	2.7462626
C	2.6921822	-3.9206734	2.8602626
O	3.3531822	-2.8916734	2.9092626
C	0.7351822	-4.4176734	1.3742626
C	1.3911822	-3.7746734	0.1982626
C	0.9591822	-4.4476734	-1.0937374
N	-0.5148178	-4.4096734	-1.2327374
C	-1.1478178	-4.7686734	-2.3387374
N	-0.4368178	-5.1356734	-3.3897374
N	-2.4908178	-4.7436734	-2.3977374
N	3.2181822	-5.1296734	2.9412626
C	4.6831822	-5.3126734	2.8222626
C	-0.3348178	-0.8616734	-5.7577374
C	-0.5438178	0.4343266	-5.2017374
C	-0.4028178	0.6923266	-3.7907374
C	-0.0798178	-0.2426734	-2.7537374
I	0.0891822	0.1683266	-0.5047374
C	0.1101822	-1.5116734	-3.3817374
C	-0.0108178	-1.8206734	-4.7857374
H	-0.5622345	1.7672857	-3.5267197
H	-0.7885036	1.3004657	-5.8241179
H	0.1844279	-2.8591774	-5.0707584
H	0.3754163	-2.3617599	-2.7449808
H	-3.4503958	8.1825204	2.3271654
H	-3.5150357	6.5892687	3.1413549
H	1.5672083	3.3792232	3.3703946
H	6.2084143	-0.6995381	5.2798234
H	7.1110353	-1.8349684	4.2642914

H	5.0058814	-5.2338390	1.7712185
H	4.9574597	-6.3005254	3.2144165
H	-6.8886081	4.4375291	3.2596837
H	-0.4217375	-1.0847448	-6.8227812
H	-4.4271818	6.8542209	1.6331064
H	-1.6494281	7.3560652	1.0745955
H	-0.2180563	5.7486442	0.1398919
H	-2.1685453	3.6032644	-0.8724774
H	-2.2117936	5.2634991	-1.4595333
H	-0.9669918	3.2634970	1.5738755
H	0.6982839	2.0567213	2.5693930
H	3.3716960	2.9259254	1.5522196
H	5.0565735	1.2461997	1.5099744
H	5.3457365	-2.0878442	4.5434538
H	5.1477580	-0.8035411	0.0611485
H	3.4353188	-1.1250046	0.3999372
H	4.5455787	1.2837057	-1.1758385
H	2.8336529	1.0592995	-0.8158462
H	4.6083702	-0.8799251	-2.3985749
H	2.8637355	-1.1193025	-2.0691995
H	-5.5628778	4.3976276	4.4536887
H	-5.1918145	4.8250229	2.7628502
H	-3.6521712	3.0711016	2.6585345
H	-4.6647384	0.3310793	3.1590450
H	-4.1031234	-0.4558968	0.9363922
H	-5.3715271	0.7906073	0.9176092
H	-2.4242864	1.1726343	0.0781258
H	-3.5502519	2.5062182	0.3015521
H	-3.3759683	1.8580609	-2.0736094
H	-5.0592644	1.6793588	-1.4766909
H	-3.7841326	1.3173244	-3.9243792
H	-3.3861523	0.0325879	-4.9927639
H	-3.7319918	-2.5352781	-2.6394029
H	-3.9494494	-2.1991310	-4.3177035
H	-4.3691087	-0.7995166	-1.1630453
H	-2.8070941	-1.1514481	3.4551448
H	-0.0595540	-0.0009028	3.1630946
H	1.4739841	-1.7174852	2.8328457
H	0.6972163	-4.4586414	3.5267071
H	2.6235058	-5.9491407	2.9772408
H	5.1939705	-4.5345579	3.4040517
H	0.9235748	-5.5060758	1.3707603
H	-0.3636188	-4.3003338	1.3654099
H	2.4885435	-3.8571630	0.2592962
H	1.1611715	-2.6966026	0.1594944
H	1.4119566	-3.9257738	-1.9544935
H	1.2842586	-5.5030554	-1.1114038
H	-1.0478797	-4.0581112	-0.4420713
H	0.5747884	-5.1305211	-3.3705461
H	-0.8722763	-5.5030395	-4.2286012
H	-2.9508609	-5.2128716	-3.1736453

H	-2.9995089	-4.8303986	-1.5204192
H	-0.6093573	-0.4663377	4.7814933
H	3.9782464	-1.1490713	2.9336428
H	3.8160899	-1.5448579	-5.8994116
H	4.0434899	-1.8558081	-4.2236073
H	2.8505344	0.5131377	-6.6027932
H	2.6397143	1.7763018	-5.4429325
H	2.9377781	1.3730712	-3.2271163

4OC1-two wall receptor

C	6.13718220	-1.33967340	4.38626260
C	5.89918220	-0.44067340	3.18126260
O	6.79318220	0.29432660	2.78226260
N	4.67618220	-0.47867340	2.63026260
C	4.29618220	0.45532660	1.56826260
C	2.92718220	0.96532660	2.04426260
O	2.10318220	0.17732660	2.51726260
C	4.17318220	-0.31867340	0.23826260
C	3.77418220	0.51532660	-0.99273740
C	3.65118220	-0.35667340	-2.22173740
N	3.32118220	0.44332660	-3.40473740
C	3.28718220	-0.00967340	-4.65573740
N	3.62118220	-1.27967340	-4.94073740
N	2.95518220	0.83232660	-5.64773740
N	2.70818220	2.27532660	1.96726260
C	1.42718220	2.85732660	2.40826260
C	0.96518220	3.89032660	1.38326260
O	1.75718220	4.70332660	0.91726260
N	-0.32881780	3.88032660	1.06926260
C	-0.97281780	4.96932660	0.30326260
C	-2.16181780	5.38132660	1.12926260
O	-2.93981780	4.54032660	1.52726260
N	-2.32981780	6.67632660	1.39226260
C	-3.49381780	7.09732660	2.16526260
C	-5.82781780	4.19732660	3.40226260
C	-5.61881780	2.71832660	3.10426260
O	-6.56581780	1.90732660	3.15426260
N	-4.37281780	2.36532660	2.82126260
C	-4.02581780	0.97332660	2.53326260
C	-2.52981780	0.82232660	2.92826260
O	-1.77281780	1.79732660	2.91026260
C	-4.28881780	0.63232660	1.06526260
C	-3.48681780	1.43432660	0.05926260
C	-4.03581780	1.27232660	-1.41073740
N	-4.03881780	-0.12567340	-1.84773740
C	-3.91081780	-0.54967340	-3.11073740
N	-3.79981780	0.31832660	-4.11173740
N	-3.96381780	-1.86667340	-3.36173740
N	-2.14381780	-0.39967340	3.28926260
C	-0.73981780	-0.66767340	3.70326260
C	-0.43981780	-2.14467340	3.44726260

O	-1.31781780	-2.99167340	3.64126260
N	0.76618220	-2.45167340	2.96026260
C	1.17618220	-3.84467340	2.74626260
C	2.69218220	-3.92067340	2.86026260
O	3.35318220	-2.89167340	2.90926260
N	3.21818220	-5.12967340	2.94126260
C	4.68318220	-5.31267340	2.82226260
C	-0.33481780	-0.86167340	-5.75773740
C	-0.54381780	0.43432660	-5.20173740
C	-0.40281780	0.69232660	-3.79073740
C	-0.07981780	-0.24267340	-2.75373740
I	0.08918220	0.16832660	-0.50473740
C	0.11018220	-1.51167340	-3.38173740
C	-0.01081780	-1.82067340	-4.78573740
H	-0.56223450	1.76728570	-3.52671970
H	-0.78850360	1.30046570	-5.82411790
H	0.18442790	-2.85917740	-5.07075840
H	0.37541630	-2.36175990	-2.74498080
H	-3.45039580	8.18252040	2.32716540
H	-3.51503570	6.58926870	3.14135490
H	1.56720830	3.37922320	3.37039460
H	6.20841430	-0.69953810	5.27982340
H	7.11103530	-1.83496840	4.26429140
H	5.00588140	-5.23383900	1.77121850
H	4.95745970	-6.30052540	3.21441650
H	-6.88860810	4.43752910	3.25968370
H	-0.42173750	-1.08474480	-6.82278120
H	-4.42718180	6.85422090	1.63310640
H	-1.64942810	7.35606520	1.07459550
H	-0.21805630	5.74864420	0.13989190
H	-0.96699180	3.26349700	1.57387550
H	0.69828390	2.05672130	2.56939300
H	3.37169600	2.92592540	1.55221960
H	5.05657350	1.24619970	1.50997440
H	5.34573650	-2.08784420	4.54345380
H	5.14775800	-0.80354110	0.06114850
H	3.43531880	-1.12500460	0.39993720
H	4.54557870	1.28370570	-1.17583850
H	2.83365290	1.05929950	-0.81584620
H	4.60837020	-0.87992510	-2.39857490
H	2.86373550	-1.11930250	-2.06919950
H	-5.56287780	4.39762760	4.45368870
H	-5.19181450	4.82502290	2.76285020
H	-3.65217120	3.07110160	2.65853450
H	-4.66473840	0.33107930	3.15904500
H	-4.10312340	-0.45589680	0.93639220
H	-5.37152710	0.79060730	0.91760920
H	-2.42428640	1.17263430	0.07812580
H	-3.55025190	2.50621820	0.30155210
H	-3.37596830	1.85806090	-2.07360940
H	-5.05926440	1.67935880	-1.47669090

H	-3.78413260	1.31732440	-3.92437920
H	-3.38615230	0.03258790	-4.99276390
H	-3.73199180	-2.53527810	-2.63940290
H	-3.94944940	-2.19913100	-4.31770350
H	-4.36910870	-0.79951660	-1.16304530
H	-2.80709410	-1.15144810	3.45514480
H	-0.05955400	-0.00090280	3.16309460
H	1.47398410	-1.71748520	2.83284570
H	0.69721630	-4.45864140	3.52670710
H	2.62350580	-5.94914070	2.97724080
H	5.19397050	-4.53455790	3.40405170
H	-0.60935730	-0.46633770	4.78149330
H	3.97824640	-1.14907130	2.93364280
H	3.81608990	-1.54485790	-5.89941160
H	4.04348990	-1.85580810	-4.22360730
H	2.85053440	0.51313770	-6.60279320
H	2.63971430	1.77630180	-5.44293250
H	2.93777810	1.37307120	-3.22711630
H	-1.37045287	4.63645521	-0.63267703
H	0.87192048	-4.24000665	1.79967059

4OC1-no wall receptor

C	6.13718220	-1.33967340	4.38626260
C	5.89918220	-0.44067340	3.18126260
O	6.79318220	0.29432660	2.78226260
N	4.67618220	-0.47867340	2.63026260
C	4.29618220	0.45532660	1.56826260
C	2.92718220	0.96532660	2.04426260
O	2.10318220	0.17732660	2.51726260
N	2.70818220	2.27532660	1.96726260
C	1.42718220	2.85732660	2.40826260
C	0.96518220	3.89032660	1.38326260
O	1.75718220	4.70332660	0.91726260
N	-0.32881780	3.88032660	1.06926260
C	-0.97281780	4.96932660	0.30326260
C	-2.16181780	5.38132660	1.12926260
O	-2.93981780	4.54032660	1.52726260
N	-2.32981780	6.67632660	1.39226260
C	-3.49381780	7.09732660	2.16526260
C	-5.82781780	4.19732660	3.40226260
C	-5.61881780	2.71832660	3.10426260
O	-6.56581780	1.90732660	3.15426260
N	-4.37281780	2.36532660	2.82126260
C	-4.02581780	0.97332660	2.53326260
C	-2.52981780	0.82232660	2.92826260
O	-1.77281780	1.79732660	2.91026260
N	-2.14381780	-0.39967340	3.28926260
C	-0.73981780	-0.66767340	3.70326260
C	-0.43981780	-2.14467340	3.44726260
O	-1.31781780	-2.99167340	3.64126260
N	0.76618220	-2.45167340	2.96026260

C	1.17618220	-3.84467340	2.74626260
C	2.69218220	-3.92067340	2.86026260
O	3.35318220	-2.89167340	2.90926260
N	3.21818220	-5.12967340	2.94126260
C	4.68318220	-5.31267340	2.82226260
C	-0.33481780	-0.86167340	-5.75773740
C	-0.54381780	0.43432660	-5.20173740
C	-0.40281780	0.69232660	-3.79073740
C	-0.07981780	-0.24267340	-2.75373740
I	0.08918220	0.16832660	-0.50473740
C	0.11018220	-1.51167340	-3.38173740
C	-0.01081780	-1.82067340	-4.78573740
H	-0.56223450	1.76728570	-3.52671970
H	-0.78850360	1.30046570	-5.82411790
H	0.18442790	-2.85917740	-5.07075840
H	0.37541630	-2.36175990	-2.74498080
H	-3.45039580	8.18252040	2.32716540
H	-3.51503570	6.58926870	3.14135490
H	1.56720830	3.37922320	3.37039460
H	6.20841430	-0.69953810	5.27982340
H	7.11103530	-1.83496840	4.26429140
H	5.00588140	-5.23383900	1.77121850
H	4.95745970	-6.30052540	3.21441650
H	-6.88860810	4.43752910	3.25968370
H	-0.42173750	-1.08474480	-6.82278120
H	-4.42718180	6.85422090	1.63310640
H	-1.64942810	7.35606520	1.07459550
H	-0.21805630	5.74864420	0.13989190
H	-0.96699180	3.26349700	1.57387550
H	0.69828390	2.05672130	2.56939300
H	3.37169600	2.92592540	1.55221960
H	5.05657350	1.24619970	1.50997440
H	5.34573650	-2.08784420	4.54345380
H	-5.56287780	4.39762760	4.45368870
H	-5.19181450	4.82502290	2.76285020
H	-3.65217120	3.07110160	2.65853450
H	-4.66473840	0.33107930	3.15904500
H	-2.80709410	-1.15144810	3.45514480
H	-0.05955400	-0.00090280	3.16309460
H	1.47398410	-1.71748520	2.83284570
H	0.69721630	-4.45864140	3.52670710
H	2.62350580	-5.94914070	2.97724080
H	5.19397050	-4.53455790	3.40405170
H	-0.60935730	-0.46633770	4.78149330
H	3.97824640	-1.14907130	2.93364280
H	-1.37045287	4.63645521	-0.63267703
H	-4.20976264	0.73482777	1.50652865
H	0.87192048	-4.24000665	1.79967059
H	4.21092770	-0.08115292	0.64640502

4OC2-four wall receptor

C	6.21603860	-1.31950890	4.26749470
C	5.93603860	-0.42050890	3.04549470
O	6.82003860	0.34549110	2.63049470
N	4.71703860	-0.48250890	2.52049470
C	4.27703860	0.42449110	1.44649470
C	2.93903860	0.98749110	1.92549470
O	2.10203860	0.22249110	2.37149470
C	4.08403860	-0.36750890	0.14249470
C	3.79703860	0.49049110	-1.12050530
C	3.65803860	-0.39050890	-2.40550530
N	3.31503860	0.44149110	-3.58350530
C	3.24603860	-0.00650890	-4.84550530
N	3.52203860	-1.29350890	-5.12750530
N	2.90903860	0.83349110	-5.84450530
N	2.72103860	2.29549110	1.80249470
C	1.44703860	2.88649110	2.25849470
C	0.99703860	3.91849110	1.24749470
O	1.79603860	4.69849110	0.74049470
N	-0.28896140	3.89049110	0.91449470
C	-0.94896140	4.93949110	0.11749470
C	-2.13996140	5.38349110	0.95249470
O	-2.92996140	4.55849110	1.37549470
C	-1.52996140	4.39049110	-1.21250530
C	-0.46996140	4.12149110	-2.30050530
O	0.71403860	4.08649110	-1.99250530
O	-0.85696140	3.92649110	-3.48150530
N	-2.31596140	6.67849110	1.18149470
C	-3.46796140	7.11849110	1.99949470
C	-5.77296140	4.17649110	3.24949470
C	-5.59196140	2.69849110	2.95249470
O	-6.55096140	1.91149110	2.99249470
N	-4.34796140	2.35749110	2.63149470
C	-3.97496140	0.95449110	2.37249470
C	-2.51896140	0.82149110	2.78549470
O	-1.79296140	1.79749110	2.77249470
C	-4.22296140	0.58949110	0.89249470
C	-3.43296140	1.45749110	-0.07950530
C	-3.89596140	1.26749110	-1.53850530
N	-3.94596140	-0.13650890	-1.91650530
C	-3.91296140	-0.58850890	-3.17950530
N	-3.97896140	-1.90150890	-3.38050530
N	-3.86196140	0.26049110	-4.22750530
N	-2.14296140	-0.37850890	3.21349470
C	-0.74196140	-0.65650890	3.58149470
C	-0.44196140	-2.11650890	3.32349470
O	-1.30496140	-2.99350890	3.54249470
N	0.77603860	-2.39050890	2.85949470
C	1.20803860	-3.80950890	2.68849470
C	2.70703860	-3.89950890	2.75749470
O	3.38103860	-2.88250890	2.75549470

C	0.70603860	-4.37850890	1.33849470
C	1.36203860	-3.72350890	0.13549470
C	1.00003860	-4.42950890	-1.18250530
N	-0.46596140	-4.37450890	-1.38750530
C	-1.07496140	-4.71650890	-2.51250530
N	-0.36496140	-5.11550890	-3.58550530
N	-2.41596140	-4.64650890	-2.56850530
N	3.23403860	-5.12650890	2.81149470
C	4.68203860	-5.29950890	2.68549470
C	-0.16496140	-1.77550890	-4.77650530
C	-0.06696140	-1.50450890	-3.37650530
C	-0.15596140	-0.22650890	-2.77850530
I	-0.00396140	0.08449110	-0.54050530
C	-0.35296140	0.76549110	-3.78650530
C	-0.47096140	0.51949110	-5.19550530
C	-0.34796140	-0.79050890	-5.75250530
H	5.51690090	-2.16583660	4.35130680
H	3.26506790	-1.09015670	0.30205840
H	5.00609470	-0.95104730	-0.01664010
H	2.87695940	1.08392560	-0.98922310
H	4.62127050	1.20619150	-1.27684870
H	2.86229930	-1.14275590	-2.25428190
H	4.61299890	-0.91015420	-2.59564830
H	2.95850590	1.37905760	-3.39014260
H	3.94923790	-1.87415870	-4.41671630
H	3.69526310	-1.56877580	-6.08773700
H	2.63253530	1.79109120	-5.64586290
H	2.78388580	0.50486410	-6.79373180
H	5.05320410	1.19445030	1.33099270
H	0.71146270	2.09052970	2.41265240
H	-2.07025170	3.45940510	-0.99827040
H	-2.27418360	5.09654980	-1.61761650
H	-0.20683750	5.72148880	-0.08573580
H	-4.41405810	6.85771100	1.50156580
H	-5.52937330	4.37024560	4.30767670
H	-5.11128010	4.79416640	2.62688300
H	-3.97013150	-0.48515920	0.76910640
H	-5.30924890	0.69820410	0.73148860
H	-3.57834490	2.51770270	0.17432470
H	-2.35994440	1.26827160	0.00401970
H	-4.89829750	1.71362950	-1.67087850
H	-3.19236260	1.79977160	-2.20311590
H	-4.25701450	-0.78330740	-1.19750180
H	-3.83989070	1.26399000	-4.06888610
H	-3.50417570	-0.05739120	-5.12149580
H	-3.69444090	-2.54466740	-2.65497700
H	-4.06689930	-2.27138160	-4.31867740
H	-4.62766270	0.32126860	2.99387240
H	-0.08823930	-0.00508530	2.99016100
H	0.88925160	-5.46735620	1.31904320
H	-0.39005930	-4.24446210	1.35078420

H	2.45942510	-3.76293030	0.22358240
H	1.09392670	-2.65744150	0.07351100
H	1.31811740	-5.48591920	-1.16612160
H	1.49645440	-3.91789460	-2.02541670
H	-1.02018680	-3.98581430	-0.62882600
H	0.64681760	-5.14409150	-3.56087680
H	-0.81838830	-5.50055510	-4.40655390
H	-2.92075480	-4.77329380	-1.69337850
H	-2.88852310	-5.07294870	-3.36154050
H	0.73432930	-4.39439450	3.49378340
H	5.19113930	-5.19475850	3.65750670
H	-0.05963630	-2.82432280	-5.07237230
H	0.09652930	-2.36707460	-2.72915430
H	-0.45278290	1.84433540	-3.52706100
H	-0.62985080	1.40498510	-5.81880600
H	1.59914200	3.39077770	3.22881980
H	6.13734450	-0.69825800	5.17384830
H	7.25112300	-1.67931930	4.19713540
H	-3.44683090	6.62670380	2.98312490
H	-3.41660720	8.20693370	2.13183800
H	-6.82501510	4.44280470	3.08666970
H	4.89943040	-6.29675790	2.27815320
H	5.07917200	-4.52603200	2.01469030
H	-0.41407950	-1.00189360	-6.82121170
H	3.39696810	2.94256810	1.40291580
H	4.04323230	-1.17102560	2.83878320
H	-0.92634710	3.28267590	1.43096940
H	-1.63584810	7.35611840	0.85764900
H	2.64405880	-5.93455100	2.97173110
H	1.47064560	-1.64539310	2.72263850
H	-3.62914600	3.06783790	2.48495680
H	-2.80108950	-1.14164440	3.34397470
H	-0.60401253	-0.44337790	4.62093940

4OC2-two wall receptor

C	6.21603860	-1.31950890	4.26749470
C	5.93603860	-0.42050890	3.04549470
O	6.82003860	0.34549110	2.63049470
N	4.71703860	-0.48250890	2.52049470
C	4.27703860	0.42449110	1.44649470
C	2.93903860	0.98749110	1.92549470
O	2.10203860	0.22249110	2.37149470
C	4.08403860	-0.36750890	0.14249470
C	3.79703860	0.49049110	-1.12050530
C	3.65803860	-0.39050890	-2.40550530
N	3.31503860	0.44149110	-3.58350530
C	3.24603860	-0.00650890	-4.84550530
N	3.52203860	-1.29350890	-5.12750530
N	2.90903860	0.83349110	-5.84450530
N	2.72103860	2.29549110	1.80249470
C	1.44703860	2.88649110	2.25849470

C	0.99703860	3.91849110	1.24749470
O	1.79603860	4.69849110	0.74049470
N	-0.28896140	3.89049110	0.91449470
C	-0.94896140	4.93949110	0.11749470
C	-2.13996140	5.38349110	0.95249470
O	-2.92996140	4.55849110	1.37549470
N	-2.31596140	6.67849110	1.18149470
C	-3.46796140	7.11849110	1.99949470
C	-5.77296140	4.17649110	3.24949470
C	-5.59196140	2.69849110	2.95249470
O	-6.55096140	1.91149110	2.99249470
N	-4.34796140	2.35749110	2.63149470
C	-3.97496140	0.95449110	2.37249470
C	-2.51896140	0.82149110	2.78549470
O	-1.79296140	1.79749110	2.77249470
C	-4.22296140	0.58949110	0.89249470
C	-3.43296140	1.45749110	-0.07950530
C	-3.89596140	1.26749110	-1.53850530
N	-3.94596140	-0.13650890	-1.91650530
C	-3.91296140	-0.58850890	-3.17950530
N	-3.97896140	-1.90150890	-3.38050530
N	-3.86196140	0.26049110	-4.22750530
N	-2.14296140	-0.37850890	3.21349470
C	-0.74196140	-0.65650890	3.58149470
C	-0.44196140	-2.11650890	3.32349470
O	-1.30496140	-2.99350890	3.54249470
N	0.77603860	-2.39050890	2.85949470
C	1.20803860	-3.80950890	2.68849470
C	2.70703860	-3.89950890	2.75749470
O	3.38103860	-2.88250890	2.75549470
N	3.23403860	-5.12650890	2.81149470
C	4.68203860	-5.29950890	2.68549470
C	-0.16496140	-1.77550890	-4.77650530
C	-0.06696140	-1.50450890	-3.37650530
C	-0.15596140	-0.22650890	-2.77850530
I	-0.00396140	0.08449110	-0.54050530
C	-0.35296140	0.76549110	-3.78650530
C	-0.47096140	0.51949110	-5.19550530
C	-0.34796140	-0.79050890	-5.75250530
H	5.51690090	-2.16583660	4.35130680
H	3.26506790	-1.09015670	0.30205840
H	5.00609470	-0.95104730	-0.01664010
H	2.87695940	1.08392560	-0.98922310
H	4.62127050	1.20619150	-1.27684870
H	2.86229930	-1.14275590	-2.25428190
H	4.61299890	-0.91015420	-2.59564830
H	2.95850590	1.37905760	-3.39014260
H	3.94923790	-1.87415870	-4.41671630
H	3.69526310	-1.56877580	-6.08773700
H	2.63253530	1.79109120	-5.64586290
H	2.78388580	0.50486410	-6.79373180

H	5.05320410	1.19445030	1.33099270
H	0.71146270	2.09052970	2.41265240
H	-0.20683750	5.72148880	-0.08573580
H	-4.41405810	6.85771100	1.50156580
H	-5.52937330	4.37024560	4.30767670
H	-5.11128010	4.79416640	2.62688300
H	-3.97013150	-0.48515920	0.76910640
H	-5.30924890	0.69820410	0.73148860
H	-3.57834490	2.51770270	0.17432470
H	-2.35994440	1.26827160	0.00401970
H	-4.89829750	1.71362950	-1.67087850
H	-3.19236260	1.79977160	-2.20311590
H	-4.25701450	-0.78330740	-1.19750180
H	-3.83989070	1.26399000	-4.06888610
H	-3.50417570	-0.05739120	-5.12149580
H	-3.69444090	-2.54466740	-2.65497700
H	-4.06689930	-2.27138160	-4.31867740
H	-4.62766270	0.32126860	2.99387240
H	-0.08823930	-0.00508530	2.99016100
H	0.73432930	-4.39439450	3.49378340
H	5.19113930	-5.19475850	3.65750670
H	-0.05963630	-2.82432280	-5.07237230
H	0.09652930	-2.36707460	-2.72915430
H	-0.45278290	1.84433540	-3.52706100
H	-0.62985080	1.40498510	-5.81880600
H	1.59914200	3.39077770	3.22881980
H	6.13734450	-0.69825800	5.17384830
H	7.25112300	-1.67931930	4.19713540
H	-3.44683090	6.62670380	2.98312490
H	-3.41660720	8.20693370	2.13183800
H	-6.82501510	4.44280470	3.08666970
H	4.89943040	-6.29675790	2.27815320
H	5.07917200	-4.52603200	2.01469030
H	-0.41407950	-1.00189360	-6.82121170
H	3.39696810	2.94256810	1.40291580
H	4.04323230	-1.17102560	2.83878320
H	-0.92634710	3.28267590	1.43096940
H	-1.63584810	7.35611840	0.85764900
H	2.64405880	-5.93455100	2.97173110
H	1.47064560	-1.64539310	2.72263850
H	-3.62914600	3.06783790	2.48495680
H	-2.80108950	-1.14164440	3.34397470
H	-1.34959200	4.56092622	-0.79961148
H	0.86119083	-4.20264910	1.75573675
H	-0.60401253	-0.44337790	4.62093940

4OC2-no wall receptor

C	6.21603860	-1.31950890	4.26749470
C	5.93603860	-0.42050890	3.04549470
O	6.82003860	0.34549110	2.63049470
N	4.71703860	-0.48250890	2.52049470

C	4.27703860	0.42449110	1.44649470
C	2.93903860	0.98749110	1.92549470
O	2.10203860	0.22249110	2.37149470
N	2.72103860	2.29549110	1.80249470
C	1.44703860	2.88649110	2.25849470
C	0.99703860	3.91849110	1.24749470
O	1.79603860	4.69849110	0.74049470
N	-0.28896140	3.89049110	0.91449470
C	-0.94896140	4.93949110	0.11749470
C	-2.13996140	5.38349110	0.95249470
O	-2.92996140	4.55849110	1.37549470
N	-2.31596140	6.67849110	1.18149470
C	-3.46796140	7.11849110	1.99949470
C	-5.77296140	4.17649110	3.24949470
C	-5.59196140	2.69849110	2.95249470
O	-6.55096140	1.91149110	2.99249470
N	-4.34796140	2.35749110	2.63149470
C	-3.97496140	0.95449110	2.37249470
C	-2.51896140	0.82149110	2.78549470
O	-1.79296140	1.79749110	2.77249470
N	-2.14296140	-0.37850890	3.21349470
C	-0.74196140	-0.65650890	3.58149470
C	-0.44196140	-2.11650890	3.32349470
O	-1.30496140	-2.99350890	3.54249470
N	0.77603860	-2.39050890	2.85949470
C	1.20803860	-3.80950890	2.68849470
C	2.70703860	-3.89950890	2.75749470
O	3.38103860	-2.88250890	2.75549470
N	3.23403860	-5.12650890	2.81149470
C	4.68203860	-5.29950890	2.68549470
C	-0.16496140	-1.77550890	-4.77650530
C	-0.06696140	-1.50450890	-3.37650530
C	-0.15596140	-0.22650890	-2.77850530
I	-0.00396140	0.08449110	-0.54050530
C	-0.35296140	0.76549110	-3.78650530
C	-0.47096140	0.51949110	-5.19550530
C	-0.34796140	-0.79050890	-5.75250530
H	5.51690090	-2.16583660	4.35130680
H	5.05320410	1.19445030	1.33099270
H	0.71146270	2.09052970	2.41265240
H	-0.20683750	5.72148880	-0.08573580
H	-4.41405810	6.85771100	1.50156580
H	-5.52937330	4.37024560	4.30767670
H	-5.11128010	4.79416640	2.62688300
H	-4.62766270	0.32126860	2.99387240
H	-0.08823930	-0.00508530	2.99016100
H	0.73432930	-4.39439450	3.49378340
H	5.19113930	-5.19475850	3.65750670
H	-0.05963630	-2.82432280	-5.07237230
H	0.09652930	-2.36707460	-2.72915430
H	-0.45278290	1.84433540	-3.52706100

H	-0.62985080	1.40498510	-5.81880600
H	1.59914200	3.39077770	3.22881980
H	6.13734450	-0.69825800	5.17384830
H	7.25112300	-1.67931930	4.19713540
H	-3.44683090	6.62670380	2.98312490
H	-3.41660720	8.20693370	2.13183800
H	-6.82501510	4.44280470	3.08666970
H	4.89943040	-6.29675790	2.27815320
H	5.07917200	-4.52603200	2.01469030
H	-0.41407950	-1.00189360	-6.82121170
H	3.39696810	2.94256810	1.40291580
H	4.04323230	-1.17102560	2.83878320
H	-0.92634710	3.28267590	1.43096940
H	-1.63584810	7.35611840	0.85764900
H	2.64405880	-5.93455100	2.97173110
H	1.47064560	-1.64539310	2.72263850
H	-3.62914600	3.06783790	2.48495680
H	-2.80108950	-1.14164440	3.34397470
H	-1.34959200	4.56092622	-0.79961148
H	0.86119083	-4.20264910	1.75573675
H	-4.14678370	0.70160748	1.34710357
H	4.14275220	-0.12657019	0.53919177
H	-0.60401253	-0.44337790	4.62093940

4OC3-four wall receptor

C	6.1889268	-1.3127086	4.3610256
C	5.9139268	-0.4097086	3.1520256
O	6.7929268	0.3462914	2.7560256
N	4.6949268	-0.4517086	2.6200256
C	4.2779268	0.4442914	1.5230256
C	2.9429268	0.9662914	2.0110256
O	2.0899268	0.1762914	2.4700256
C	4.1959268	-0.3407086	0.1810256
C	3.6849268	0.4742914	-1.0379744
C	3.7859268	-0.3677086	-2.3349744
N	3.4109268	0.4422914	-3.4859744
C	3.3339268	-0.0057086	-4.7399744
N	3.6789268	-1.2767086	-5.0109744
N	2.9369268	0.8222914	-5.7239744
N	2.7369268	2.2832914	1.9400256
C	1.4489268	2.8542914	2.3710256
C	0.9899268	3.9092914	1.3510256
O	1.7909268	4.6882914	0.8570256
N	-0.2890732	3.9022914	1.0300256
C	-0.9590732	4.9772914	0.2740256
C	-2.1500732	5.4132914	1.1390256
O	-2.9770732	4.5822914	1.5360256
C	-1.5770732	4.4582914	-1.0879744
C	-0.5340732	4.1832914	-2.1869744
O	0.6609268	4.2042914	-1.8949744
O	-0.9340732	3.9122914	-3.3589744

N	-2.3330732	6.7082914	1.3650256
C	-3.5200732	7.0952914	2.1390256
C	-5.8520732	4.1852914	3.4360256
C	-5.6420732	2.7072914	3.0950256
O	-6.5860732	1.8892914	3.1440256
N	-4.4030732	2.3532914	2.8280256
C	-4.0460732	0.9422914	2.6030256
C	-2.5350732	0.7912914	2.9570256
O	-1.8140732	1.7692914	2.9360256
C	-4.2900732	0.5642914	1.1540256
C	-3.4290732	1.3512914	0.1390256
C	-4.0400732	1.2722914	-1.3139744
N	-4.0770732	-0.1257086	-1.7559744
C	-3.9700732	-0.5537086	-3.0329744
N	-4.0440732	-1.8747086	-3.2799744
N	-3.7810732	0.2992914	-4.0529744
N	-2.0950732	-0.4267086	3.2870256
C	-0.6910732	-0.6607086	3.7090256
C	-0.4080732	-2.1257086	3.4290256
O	-1.2870732	-2.9747086	3.6830256
N	0.7859268	-2.4227086	2.9480256
C	1.1809268	-3.8257086	2.7440256
C	2.6929268	-3.9157086	2.8350256
O	3.3669268	-2.8957086	2.8500256
C	0.6669268	-4.3487086	1.3800256
C	1.4389268	-3.7987086	0.1820256
C	0.9339268	-4.4337086	-1.1359744
N	-0.5260732	-4.4447086	-1.2519744
C	-1.2010732	-4.7667086	-2.3539744
N	-0.5450732	-5.1037086	-3.4689744
N	-2.5280732	-4.7617086	-2.3389744
N	3.2349268	-5.1267086	2.9270256
C	4.6789268	-5.3107086	2.8040256
C	-0.0710732	-1.8007086	-4.7199744
C	0.0219268	-1.5247086	-3.3079744
C	-0.1170732	-0.2567086	-2.6849744
I	0.0199268	0.0942914	-0.4559744
C	-0.3530732	0.7362914	-3.6619744
C	-0.4650732	0.4922914	-5.0659744
C	-0.2950732	-0.7877086	-5.6589744
H	5.4148129	-2.0767439	4.5298509
H	3.5413410	-1.2145362	0.3468725
H	5.2107887	-0.7214910	-0.0176343
H	2.6558669	0.8241518	-0.8915040
H	4.3150774	1.3729197	-1.1608187
H	3.1131003	-1.2430149	-2.2650938
H	4.8226335	-0.7302692	-2.4551442
H	3.0771607	1.3875926	-3.2960866
H	4.1986174	-1.8092815	-4.3240790
H	3.7769936	-1.5781812	-5.9736192
H	2.5721255	1.7461401	-5.5091649

H	2.8787635	0.5159447	-6.6870788
H	5.0315288	1.2415379	1.4487168
H	0.7197458	2.0495944	2.5085686
H	-2.1404599	3.5376445	-0.8779044
H	-2.3087302	5.1939579	-1.4620056
H	-0.2187408	5.7609344	0.0730988
H	-4.4350211	6.7726061	1.6203859
H	-5.6975895	4.3200099	4.5191353
H	-5.1443265	4.8281379	2.8952137
H	-4.1154839	-0.5277117	1.0458634
H	-5.3640254	0.7408074	0.9704236
H	-3.4119242	2.4153974	0.4208620
H	-2.3963134	1.0015548	0.1183646
H	-5.0561674	1.6990521	-1.3313664
H	-3.3942030	1.8560876	-1.9909729
H	-4.3725350	-0.7992678	-1.0558085
H	-3.5967600	1.2829351	-3.8644547
H	-3.4193945	-0.0455103	-4.9360016
H	-4.3943743	-2.4819764	-2.5498172
H	-4.2575785	-2.1757253	-4.2249585
H	-4.6814463	0.3217577	3.2533969
H	-0.0171114	0.0176746	3.1764864
H	0.7147689	-5.4531246	1.3758310
H	-0.4037144	-4.0812576	1.3628666
H	2.5110785	-4.0321192	0.2580056
H	1.3407044	-2.7021511	0.1390233
H	1.2909830	-5.4780741	-1.1949271
H	1.3629308	-3.8809058	-1.9894942
H	-1.0504612	-4.1374834	-0.4373301
H	-3.0119404	-4.7749161	-1.4463475
H	-3.0445181	-5.1713750	-3.1103652
H	0.4663692	-5.1252526	-3.4951130
H	-1.0324789	-5.4377194	-4.2922381
H	0.7009460	-4.4248666	3.5348725
H	5.1995382	-4.5150458	3.3531507
H	0.0666940	-2.8406619	-5.0296451
H	0.2047203	-2.3895533	-2.6677697
H	-0.4910128	1.8079444	-3.3912369
H	-0.6563582	1.3795251	-5.6789790
H	6.2622756	-0.6703700	5.2522548
H	1.5722558	3.3585141	3.3450780
H	-3.5038051	6.6252052	3.1334503
H	-3.5362040	8.1872945	2.2542914
H	-6.8888459	4.4571080	3.2004275
H	4.9615739	-6.2834138	3.2279400
H	5.0018852	-5.2706092	1.7497537
H	-0.3615166	-0.9619892	-6.7345786
H	2.6389179	-5.9454854	2.9747849
H	4.0184791	-1.1491225	2.9140672
H	3.4010951	2.9330678	1.5245079
H	-0.9263731	3.2877527	1.5386430

H	-1.6499667	7.3963476	1.0712328
H	-3.6685562	3.0502873	2.6907529
H	-2.7343674	-1.1946317	3.4746534
H	1.4868757	-1.6856641	2.7934040
H	-0.5693643	-0.4782330	4.7914836
H	7.1694149	-1.7881003	4.2180094

4OC3-two wall receptor

C	6.18892680	-1.31270860	4.36102560
C	5.91392680	-0.40970860	3.15202560
O	6.79292680	0.34629140	2.75602560
N	4.69492680	-0.45170860	2.62002560
C	4.27792680	0.44429140	1.52302560
C	2.94292680	0.96629140	2.01102560
O	2.08992680	0.17629140	2.47002560
C	4.19592680	-0.34070860	0.18102560
C	3.68492680	0.47429140	-1.03797440
C	3.78592680	-0.36770860	-2.33497440
N	3.41092680	0.44229140	-3.48597440
C	3.33392680	-0.00570860	-4.73997440
N	3.67892680	-1.27670860	-5.01097440
N	2.93692680	0.82229140	-5.72397440
N	2.73692680	2.28329140	1.94002560
C	1.44892680	2.85429140	2.37102560
C	0.98992680	3.90929140	1.35102560
O	1.79092680	4.68829140	0.85702560
N	-0.28907320	3.90229140	1.03002560
C	-0.95907320	4.97729140	0.27402560
C	-2.15007320	5.41329140	1.13902560
O	-2.97707320	4.58229140	1.53602560
N	-2.33307320	6.70829140	1.36502560
C	-3.52007320	7.09529140	2.13902560
C	-5.85207320	4.18529140	3.43602560
C	-5.64207320	2.70729140	3.09502560
O	-6.58607320	1.88929140	3.14402560
N	-4.40307320	2.35329140	2.82802560
C	-4.04607320	0.94229140	2.60302560
C	-2.53507320	0.79129140	2.95702560
O	-1.81407320	1.76929140	2.93602560
C	-4.29007320	0.56429140	1.15402560
C	-3.42907320	1.35129140	0.13902560
C	-4.04007320	1.27229140	-1.31397440
N	-4.07707320	-0.12570860	-1.75597440
C	-3.97007320	-0.55370860	-3.03297440
N	-4.04407320	-1.87470860	-3.27997440
N	-3.78107320	0.29929140	-4.05297440
N	-2.09507320	-0.42670860	3.28702560
C	-0.69107320	-0.66070860	3.70902560
C	-0.40807320	-2.12570860	3.42902560
O	-1.28707320	-2.97470860	3.68302560
N	0.78592680	-2.42270860	2.94802560

C	1.18092680	-3.82570860	2.74402560
C	2.69292680	-3.91570860	2.83502560
O	3.36692680	-2.89570860	2.85002560
N	3.23492680	-5.12670860	2.92702560
C	4.67892680	-5.31070860	2.80402560
C	-0.07107320	-1.80070860	-4.71997440
C	0.02192680	-1.52470860	-3.30797440
C	-0.11707320	-0.25670860	-2.68497440
I	0.01992680	0.09429140	-0.45597440
C	-0.35307320	0.73629140	-3.66197440
C	-0.46507320	0.49229140	-5.06597440
C	-0.29507320	-0.78770860	-5.65897440
H	5.41481290	-2.07674390	4.52985090
H	3.54134100	-1.21453620	0.34687250
H	5.21078870	-0.72149100	-0.01763430
H	2.65586690	0.82415180	-0.89150400
H	4.31507740	1.37291970	-1.16081870
H	3.11310030	-1.24301490	-2.26509380
H	4.82263350	-0.73026920	-2.45514420
H	3.07716070	1.38759260	-3.29608660
H	4.19861740	-1.80928150	-4.32407900
H	3.77699360	-1.57818120	-5.97361920
H	2.57212550	1.74614010	-5.50916490
H	2.87876350	0.51594470	-6.68707880
H	5.03152880	1.24153790	1.44871680
H	0.71974580	2.04959440	2.50856860
H	-0.21874080	5.76093440	0.07309880
H	-4.43502110	6.77260610	1.62038590
H	-5.69758950	4.32000990	4.51913530
H	-5.14432650	4.82813790	2.89521370
H	-4.11548390	-0.52771170	1.04586340
H	-5.36402540	0.74080740	0.97042360
H	-3.41192420	2.41539740	0.42086200
H	-2.39631340	1.00155480	0.11836460
H	-5.05616740	1.69905210	-1.33136640
H	-3.39420300	1.85608760	-1.99097290
H	-4.37253500	-0.79926780	-1.05580850
H	-3.59676000	1.28293510	-3.86445470
H	-3.41939450	-0.04551030	-4.93600160
H	-4.39437430	-2.48197640	-2.54981720
H	-4.25757850	-2.17572530	-4.22495850
H	-4.68144630	0.32175770	3.25339690
H	-0.01711140	0.01767460	3.17648640
H	0.70094600	-4.42486660	3.53487250
H	5.19953820	-4.51504580	3.35315070
H	0.06669400	-2.84066190	-5.02964510
H	0.20472030	-2.38955330	-2.66776970
H	-0.49101280	1.80794440	-3.39123690
H	-0.65635820	1.37952510	-5.67897900
H	6.26227560	-0.67037000	5.25225480
H	1.57225580	3.35851410	3.34507800

H	-3.50380510	6.62520520	3.13345030
H	-3.53620400	8.18729450	2.25429140
H	-6.88884590	4.45710800	3.20042750
H	4.96157390	-6.28341380	3.22794000
H	5.00188520	-5.27060920	1.74975370
H	-0.36151660	-0.96198920	-6.73457860
H	2.63891790	-5.94548540	2.97478490
H	4.01847910	-1.14912250	2.91406720
H	3.40109510	2.93306780	1.52450790
H	-0.92637310	3.28775270	1.53864300
H	-1.64996670	7.39634760	1.07123280
H	-3.66855620	3.05028730	2.69075290
H	-2.73436740	-1.19463170	3.47465340
H	1.48687570	-1.68566410	2.79340400
H	-0.56936430	-0.47823300	4.79148360
H	7.16941490	-1.78810030	4.21800940
H	-1.37676237	4.62651360	-0.64651266
H	0.82578459	-4.18706926	1.80158595

4OC3-no wall receptor

C	6.18892680	-1.31270860	4.36102560
C	5.91392680	-0.40970860	3.15202560
O	6.79292680	0.34629140	2.75602560
N	4.69492680	-0.45170860	2.62002560
C	4.27792680	0.44429140	1.52302560
C	2.94292680	0.96629140	2.01102560
O	2.08992680	0.17629140	2.47002560
N	2.73692680	2.28329140	1.94002560
C	1.44892680	2.85429140	2.37102560
C	0.98992680	3.90929140	1.35102560
O	1.79092680	4.68829140	0.85702560
N	-0.28907320	3.90229140	1.03002560
C	-0.95907320	4.97729140	0.27402560
C	-2.15007320	5.41329140	1.13902560
O	-2.97707320	4.58229140	1.53602560
N	-2.33307320	6.70829140	1.36502560
C	-3.52007320	7.09529140	2.13902560
C	-5.85207320	4.18529140	3.43602560
C	-5.64207320	2.70729140	3.09502560
O	-6.58607320	1.88929140	3.14402560
N	-4.40307320	2.35329140	2.82802560
C	-4.04607320	0.94229140	2.60302560
C	-2.53507320	0.79129140	2.95702560
O	-1.81407320	1.76929140	2.93602560
N	-2.09507320	-0.42670860	3.28702560
C	-0.69107320	-0.66070860	3.70902560
C	-0.40807320	-2.12570860	3.42902560
O	-1.28707320	-2.97470860	3.68302560
N	0.78592680	-2.42270860	2.94802560
C	1.18092680	-3.82570860	2.74402560
C	2.69292680	-3.91570860	2.83502560

O	3.36692680	-2.89570860	2.85002560
N	3.23492680	-5.12670860	2.92702560
C	4.67892680	-5.31070860	2.80402560
C	-0.07107320	-1.80070860	-4.71997440
C	0.02192680	-1.52470860	-3.30797440
C	-0.11707320	-0.25670860	-2.68497440
I	0.01992680	0.09429140	-0.45597440
C	-0.35307320	0.73629140	-3.66197440
C	-0.46507320	0.49229140	-5.06597440
C	-0.29507320	-0.78770860	-5.65897440
H	5.41481290	-2.07674390	4.52985090
H	5.03152880	1.24153790	1.44871680
H	0.71974580	2.04959440	2.50856860
H	-0.21874080	5.76093440	0.07309880
H	-4.43502110	6.77260610	1.62038590
H	-5.69758950	4.32000990	4.51913530
H	-5.14432650	4.82813790	2.89521370
H	-4.68144630	0.32175770	3.25339690
H	-0.01711140	0.01767460	3.17648640
H	0.70094600	-4.42486660	3.53487250
H	5.19953820	-4.51504580	3.35315070
H	0.06669400	-2.84066190	-5.02964510
H	0.20472030	-2.38955330	-2.66776970
H	-0.49101280	1.80794440	-3.39123690
H	-0.65635820	1.37952510	-5.67897900
H	6.26227560	-0.67037000	5.25225480
H	1.57225580	3.35851410	3.34507800
H	-3.50380510	6.62520520	3.13345030
H	-3.53620400	8.18729450	2.25429140
H	-6.88884590	4.45710800	3.20042750
H	4.96157390	-6.28341380	3.22794000
H	5.00188520	-5.27060920	1.74975370
H	-0.36151660	-0.96198920	-6.73457860
H	2.63891790	-5.94548540	2.97478490
H	4.01847910	-1.14912250	2.91406720
H	3.40109510	2.93306780	1.52450790
H	-0.92637310	3.28775270	1.53864300
H	-1.64996670	7.39634760	1.07123280
H	-3.66855620	3.05028730	2.69075290
H	-2.73436740	-1.19463170	3.47465340
H	1.48687570	-1.68566410	2.79340400
H	-0.56936430	-0.47823300	4.79148360
H	7.16941490	-1.78810030	4.21800940
H	-1.37676237	4.62651360	-0.64651266
H	0.82578459	-4.18706926	1.80158595
H	-4.21814867	0.67571547	1.58115119
H	4.22157094	-0.09521291	0.60071377

4OC4-four wall receptor

C	6.64171040	-1.64441710	4.20283990
C	6.40771040	-0.72241710	2.99883990

O	7.31471040	0.04058290	2.60883990
N	5.20971040	-0.81941710	2.42883990
C	4.73771040	0.06058290	1.36183990
C	3.38871040	0.62058290	1.80483990
O	2.50871040	-0.13241710	2.22483990
C	4.61671040	-0.72541710	0.04283990
C	4.31671040	0.12858290	-1.17016010
C	4.14471040	-0.72141710	-2.42216010
N	3.84871040	0.12658290	-3.57816010
C	3.81071040	-0.31341710	-4.84216010
N	4.08471040	-1.60941710	-5.13616010
N	3.55071040	0.54858290	-5.82916010
N	3.21971040	1.93858290	1.73683990
C	1.93371040	2.54158290	2.18183990
C	1.48071040	3.62058290	1.21283990
O	2.28671040	4.46758290	0.80883990
N	0.19771040	3.60158290	0.84983990
C	-0.44528960	4.70458290	0.11883990
C	-1.63328960	5.09958290	0.95283990
O	-2.40628960	4.26558290	1.34683990
C	-1.02928960	4.24958290	-1.23816010
C	0.01471040	3.82958290	-2.27216010
O	1.21771040	3.82058290	-1.99216010
O	-0.42128960	3.47358290	-3.40916010
N	-1.84028960	6.39158290	1.17583990
C	-3.00228960	6.81758290	1.97583990
C	-5.33528960	3.91058290	3.22283990
C	-5.14528960	2.44658290	2.90183990
O	-6.09428960	1.65958290	2.95183990
N	-3.89528960	2.09358290	2.63283990
C	-3.53128960	0.69358290	2.34083990
C	-2.05728960	0.52358290	2.72783990
O	-1.30828960	1.48758290	2.74083990
C	-3.78528960	0.35958290	0.85283990
C	-2.89728960	1.15358290	-0.12316010
C	-3.33328960	0.96258290	-1.58416010
N	-3.37928960	-0.45841710	-1.97916010
C	-3.35328960	-0.88741710	-3.23416010
N	-3.42728960	-2.20541710	-3.48816010
N	-3.32728960	-0.01241710	-4.23416010
N	-1.67328960	-0.70341710	3.07083990
C	-0.27228960	-0.98741710	3.45383990
C	0.01271040	-2.45641710	3.22983990
O	-0.86728960	-3.30641710	3.46283990
N	1.25171040	-2.77041710	2.86883990
C	1.67071040	-4.15641710	2.70283990
C	3.16971040	-4.24041710	2.53183990
O	3.82371040	-3.24741710	2.20283990
C	0.97771040	-4.76541710	1.49283990
C	0.48171040	-3.70841710	0.55283990
C	-0.58928960	-4.25241710	-0.30716010

N	0.00671040	-4.71141710	-1.53916010
C	-0.66828960	-5.11141710	-2.60016010
N	0.02071040	-5.47141710	-3.68516010
N	-2.01028960	-5.09341710	-2.62416010
N	3.70871040	-5.43441710	2.75083990
C	5.14971040	-5.65141710	2.63583990
C	0.19071040	0.23258290	-5.31116010
C	0.34571040	0.42758290	-3.92116010
C	0.40371040	-0.61041710	-2.98116010
I	0.58971040	-0.32841710	-0.78416010
C	0.34271040	-1.88941710	-3.55916010
C	0.21371040	-2.11741710	-4.95016010
C	0.15371040	-1.06241710	-5.85616010
H	5.96186320	-2.51108920	4.22307570
H	3.83833050	-1.49576500	0.18503160
H	5.57063460	-1.26069230	-0.09605770
H	3.40737720	0.73336900	-1.01361400
H	5.13937200	0.84534530	-1.33784290
H	3.32229440	-1.44665370	-2.27682830
H	5.07632830	-1.28265840	-2.61507510
H	3.48137850	1.05945350	-3.38440600
H	4.44920990	-2.21304500	-4.41025680
H	4.31819400	-1.86337730	-6.08951700
H	3.31149290	1.51479690	-5.62519720
H	3.42724600	0.24071820	-6.78598990
H	5.49004640	0.85723690	1.25645740
H	1.19507320	1.74500270	2.31080490
H	-1.71960760	3.41247400	-1.06707980
H	-1.63798220	5.06359340	-1.66698080
H	0.30827050	5.48746120	-0.03103320
H	-3.95285520	6.53436890	1.50213710
H	-4.88828780	4.10200990	4.21760600
H	-4.77361030	4.53976860	2.51687390
H	-3.62467300	-0.73262660	0.73143880
H	-4.85412920	0.55542590	0.66556280
H	-2.97075050	2.22745390	0.10657130
H	-1.84094060	0.88744630	-0.00627800
H	-4.33292420	1.40544150	-1.74116650
H	-2.61067010	1.49178190	-2.23296540
H	-3.64347550	-1.11855350	-1.25435970
H	-3.28699840	0.98598540	-4.04684200
H	-3.04586630	-0.29771570	-5.16551460
H	-3.10630770	-2.87004610	-2.79640540
H	-3.44528740	-2.52728710	-4.44783120
H	-4.18159390	0.04985990	2.95332760
H	0.40554850	-0.33255800	2.89527250
H	0.10704630	-5.32956980	1.85894770
H	1.63793700	-5.49289710	0.98971540
H	0.03950810	-2.88396680	1.10434730
H	1.28352360	-3.24363550	-0.04067370
H	-1.14390780	-5.06475180	0.19415350

H	-1.31203460	-3.45783680	-0.57080860
H	1.01518030	-4.82829870	-1.54458900
H	-2.50444250	-5.18435610	-1.73926290
H	-2.48718480	-5.52933100	-3.40884580
H	1.03177580	-5.41034070	-3.70928180
H	-0.42225750	-5.91128540	-4.48460450
H	1.36611660	-4.71788830	3.60199910
H	5.56071850	-4.92140310	1.92739170
H	0.11566730	1.12836880	-5.93417750
H	0.32856390	1.49721810	-3.60400270
H	0.40712960	-2.76042380	-2.90590960
H	0.18321290	-3.15361370	-5.29990120
H	-2.97907310	7.90895560	2.08856750
H	-2.97654600	6.35400770	2.97339830
H	2.08341770	3.01862380	3.16538430
H	7.68663450	-1.98117400	4.18218890
H	6.49630890	-1.06061980	5.12622740
H	5.65444570	-5.51033820	3.60591900
H	5.34778120	-6.67168400	2.27752370
H	-0.10978360	-0.77616740	4.52651410
H	0.05405080	-1.23408440	-6.93120040
H	-1.15505500	7.07552650	0.87770680
H	-0.44440190	2.96893950	1.32783820
H	3.91891920	2.58172840	1.37344630
H	4.56610680	-1.55378220	2.70689520
H	3.14103930	-6.17212810	3.15373040
H	1.93295840	-2.02898620	2.65272340
H	-2.33772690	-1.45478110	3.23546090
H	-3.17958560	2.80562370	2.45769250
H	-6.36814540	4.18941747	3.20386163

4OC4- two wall receptor

C	6.64171040	-1.64441710	4.20283990
C	6.40771040	-0.72241710	2.99883990
O	7.31471040	0.04058290	2.60883990
N	5.20971040	-0.81941710	2.42883990
C	4.73771040	0.06058290	1.36183990
C	3.38871040	0.62058290	1.80483990
O	2.50871040	-0.13241710	2.22483990
C	4.61671040	-0.72541710	0.04283990
C	4.31671040	0.12858290	-1.17016010
C	4.14471040	-0.72141710	-2.42216010
N	3.84871040	0.12658290	-3.57816010
C	3.81071040	-0.31341710	-4.84216010
N	4.08471040	-1.60941710	-5.13616010
N	3.55071040	0.54858290	-5.82916010
N	3.21971040	1.93858290	1.73683990
C	1.93371040	2.54158290	2.18183990
C	1.48071040	3.62058290	1.21283990
O	2.28671040	4.46758290	0.80883990
N	0.19771040	3.60158290	0.84983990

C	-0.44528960	4.70458290	0.11883990
C	-1.63328960	5.09958290	0.95283990
O	-2.40628960	4.26558290	1.34683990
N	-1.84028960	6.39158290	1.17583990
C	-3.00228960	6.81758290	1.97583990
C	-5.33528960	3.91058290	3.22283990
C	-5.14528960	2.44658290	2.90183990
O	-6.09428960	1.65958290	2.95183990
N	-3.89528960	2.09358290	2.63283990
C	-3.53128960	0.69358290	2.34083990
C	-2.05728960	0.52358290	2.72783990
O	-1.30828960	1.48758290	2.74083990
C	-3.78528960	0.35958290	0.85283990
C	-2.89728960	1.15358290	-0.12316010
C	-3.33328960	0.96258290	-1.58416010
N	-3.37928960	-0.45841710	-1.97916010
C	-3.35328960	-0.88741710	-3.23416010
N	-3.42728960	-2.20541710	-3.48816010
N	-3.32728960	-0.01241710	-4.23416010
N	-1.67328960	-0.70341710	3.07083990
C	-0.27228960	-0.98741710	3.45383990
C	0.01271040	-2.45641710	3.22983990
O	-0.86728960	-3.30641710	3.46283990
N	1.25171040	-2.77041710	2.86883990
C	1.67071040	-4.15641710	2.70283990
C	3.16971040	-4.24041710	2.53183990
O	3.82371040	-3.24741710	2.20283990
N	3.70871040	-5.43441710	2.75083990
C	5.14971040	-5.65141710	2.63583990
C	0.19071040	0.23258290	-5.31116010
C	0.34571040	0.42758290	-3.92116010
C	0.40371040	-0.61041710	-2.98116010
I	0.58971040	-0.32841710	-0.78416010
C	0.34271040	-1.88941710	-3.55916010
C	0.21371040	-2.11741710	-4.95016010
C	0.15371040	-1.06241710	-5.85616010
H	5.96186320	-2.51108920	4.22307570
H	3.83833050	-1.49576500	0.18503160
H	5.57063460	-1.26069230	-0.09605770
H	3.40737720	0.73336900	-1.01361400
H	5.13937200	0.84534530	-1.33784290
H	3.32229440	-1.44665370	-2.27682830
H	5.07632830	-1.28265840	-2.61507510
H	3.48137850	1.05945350	-3.38440600
H	4.44920990	-2.21304500	-4.41025680
H	4.31819400	-1.86337730	-6.08951700
H	3.31149290	1.51479690	-5.62519720
H	3.42724600	0.24071820	-6.78598990
H	5.49004640	0.85723690	1.25645740
H	1.19507320	1.74500270	2.31080490
H	0.30827050	5.48746120	-0.03103320

H	-3.95285520	6.53436890	1.50213710
H	-4.88828780	4.10200990	4.21760600
H	-4.77361030	4.53976860	2.51687390
H	-3.62467300	-0.73262660	0.73143880
H	-4.85412920	0.55542590	0.66556280
H	-2.97075050	2.22745390	0.10657130
H	-1.84094060	0.88744630	-0.00627800
H	-4.33292420	1.40544150	-1.74116650
H	-2.61067010	1.49178190	-2.23296540
H	-3.64347550	-1.11855350	-1.25435970
H	-3.28699840	0.98598540	-4.04684200
H	-3.04586630	-0.29771570	-5.16551460
H	-3.10630770	-2.87004610	-2.79640540
H	-3.44528740	-2.52728710	-4.44783120
H	-4.18159390	0.04985990	2.95332760
H	0.40554850	-0.33255800	2.89527250
H	1.36611660	-4.71788830	3.60199910
H	5.56071850	-4.92140310	1.92739170
H	0.11566730	1.12836880	-5.93417750
H	0.32856390	1.49721810	-3.60400270
H	0.40712960	-2.76042380	-2.90590960
H	0.18321290	-3.15361370	-5.29990120
H	-2.97907310	7.90895560	2.08856750
H	-2.97654600	6.35400770	2.97339830
H	2.08341770	3.01862380	3.16538430
H	7.68663450	-1.98117400	4.18218890
H	6.49630890	-1.06061980	5.12622740
H	5.65444570	-5.51033820	3.60591900
H	5.34778120	-6.67168400	2.27752370
H	-0.10978360	-0.77616740	4.52651410
H	0.05405080	-1.23408440	-6.93120040
H	-1.15505500	7.07552650	0.87770680
H	-0.44440190	2.96893950	1.32783820
H	3.91891920	2.58172840	1.37344630
H	4.56610680	-1.55378220	2.70689520
H	3.14103930	-6.17212810	3.15373040
H	1.93295840	-2.02898620	2.65272340
H	-2.33772690	-1.45478110	3.23546090
H	-3.17958560	2.80562370	2.45769250
H	-0.84953062	4.38963484	-0.82046672
H	1.18338400	-4.58467364	1.85195253
H	-6.36814540	4.18941747	3.20386163

4OC4-no wall receptor

C	6.64171040	-1.64441710	4.20283990
C	6.40771040	-0.72241710	2.99883990
O	7.31471040	0.04058290	2.60883990
N	5.20971040	-0.81941710	2.42883990
C	4.73771040	0.06058290	1.36183990
C	3.38871040	0.62058290	1.80483990
O	2.50871040	-0.13241710	2.22483990

N	3.21971040	1.93858290	1.73683990
C	1.93371040	2.54158290	2.18183990
C	1.48071040	3.62058290	1.21283990
O	2.28671040	4.46758290	0.80883990
N	0.19771040	3.60158290	0.84983990
C	-0.44528960	4.70458290	0.11883990
C	-1.63328960	5.09958290	0.95283990
O	-2.40628960	4.26558290	1.34683990
N	-1.84028960	6.39158290	1.17583990
C	-3.00228960	6.81758290	1.97583990
C	-5.33528960	3.91058290	3.22283990
C	-5.14528960	2.44658290	2.90183990
O	-6.09428960	1.65958290	2.95183990
N	-3.89528960	2.09358290	2.63283990
C	-3.53128960	0.69358290	2.34083990
C	-2.05728960	0.52358290	2.72783990
O	-1.30828960	1.48758290	2.74083990
N	-1.67328960	-0.70341710	3.07083990
C	-0.27228960	-0.98741710	3.45383990
C	0.01271040	-2.45641710	3.22983990
O	-0.86728960	-3.30641710	3.46283990
N	1.25171040	-2.77041710	2.86883990
C	1.67071040	-4.15641710	2.70283990
C	3.16971040	-4.24041710	2.53183990
O	3.82371040	-3.24741710	2.20283990
N	3.70871040	-5.43441710	2.75083990
C	5.14971040	-5.65141710	2.63583990
C	0.19071040	0.23258290	-5.31116010
C	0.34571040	0.42758290	-3.92116010
C	0.40371040	-0.61041710	-2.98116010
I	0.58971040	-0.32841710	-0.78416010
C	0.34271040	-1.88941710	-3.55916010
C	0.21371040	-2.11741710	-4.95016010
C	0.15371040	-1.06241710	-5.85616010
H	5.96186320	-2.51108920	4.22307570
H	5.49004640	0.85723690	1.25645740
H	1.19507320	1.74500270	2.31080490
H	0.30827050	5.48746120	-0.03103320
H	-3.95285520	6.53436890	1.50213710
H	-4.88828780	4.10200990	4.21760600
H	-4.77361030	4.53976860	2.51687390
H	-4.18159390	0.04985990	2.95332760
H	0.40554850	-0.33255800	2.89527250
H	1.36611660	-4.71788830	3.60199910
H	5.56071850	-4.92140310	1.92739170
H	0.11566730	1.12836880	-5.93417750
H	0.32856390	1.49721810	-3.60400270
H	0.40712960	-2.76042380	-2.90590960
H	0.18321290	-3.15361370	-5.29990120
H	-2.97907310	7.90895560	2.08856750
H	-2.97654600	6.35400770	2.97339830

H	2.08341770	3.01862380	3.16538430
H	7.68663450	-1.98117400	4.18218890
H	6.49630890	-1.06061980	5.12622740
H	5.65444570	-5.51033820	3.60591900
H	5.34778120	-6.67168400	2.27752370
H	-0.10978360	-0.77616740	4.52651410
H	0.05405080	-1.23408440	-6.93120040
H	-1.15505500	7.07552650	0.87770680
H	-0.44440190	2.96893950	1.32783820
H	3.91891920	2.58172840	1.37344630
H	4.56610680	-1.55378220	2.70689520
H	3.14103930	-6.17212810	3.15373040
H	1.93295840	-2.02898620	2.65272340
H	-2.33772690	-1.45478110	3.23546090
H	-3.17958560	2.80562370	2.45769250
H	-0.84953062	4.38963484	-0.82046672
H	1.18338400	-4.58467364	1.85195253
H	-3.70708152	0.46242344	1.31100375
H	4.65364957	-0.48546514	0.44550737
H	-6.36814540	4.18941747	3.20386163

4OC5-four wall receptor

C	6.1560702	-1.3265516	4.3825683
C	5.8980702	-0.4205516	3.1675683
O	6.7970702	0.3284484	2.7365683
N	4.6700702	-0.4945516	2.6365683
C	4.2410702	0.3854484	1.5375683
C	2.8920702	0.9394484	2.0425683
O	2.0780702	0.1824484	2.5755683
C	4.1380702	-0.4025516	0.2275683
C	3.8530702	0.4584484	-1.0204317
C	3.7050702	-0.3815516	-2.3074317
N	3.4540702	0.4764484	-3.4514317
C	3.3650702	0.0364484	-4.7124317
N	3.5990702	-1.2455516	-5.0024317
N	3.0900702	0.8844484	-5.6974317
N	2.6910702	2.2494484	1.9715683
C	1.4000702	2.8134484	2.4245683
C	0.9570702	3.8704484	1.4185683
O	1.7610702	4.6974484	0.9925683
N	-0.3359298	3.8754484	1.0775683
C	-0.9539298	4.9484484	0.2945683
C	-2.1519298	5.3634484	1.1135683
O	-2.9419298	4.5244484	1.5205683
C	-1.5109298	4.4244484	-1.0514317
C	-0.4489298	4.1264484	-2.1014317
O	0.7530702	4.1964484	-1.8384317
O	-0.8509298	3.8224484	-3.2624317
N	-2.3489298	6.6554484	1.3275683
C	-3.5269298	7.0714484	2.1085683
C	-5.8849298	4.1624484	3.3705683

C	-5.6769298	2.6844484	3.0125683
O	-6.6249298	1.8744484	3.0995683
N	-4.4149298	2.3184484	2.7755683
C	-4.0729298	0.9264484	2.5375683
C	-2.5719298	0.7984484	2.9085683
O	-1.8619298	1.7964484	2.8555683
C	-4.2889298	0.5764484	1.0635683
C	-3.4929298	1.3954484	0.0935683
C	-3.9109298	1.2224484	-1.3974317
N	-3.9779298	-0.1775516	-1.8254317
C	-3.9019298	-0.5915516	-3.0854317
N	-4.0379298	-1.9005516	-3.3414317
N	-3.7739298	0.2694484	-4.1034317
N	-2.1459298	-0.4235516	3.2375683
C	-0.7529298	-0.6765516	3.6675683
C	-0.4789298	-2.1395516	3.4065683
O	-1.3719298	-3.0135516	3.6135683
N	0.7320702	-2.4225516	2.9365683
C	1.1570702	-3.8265516	2.7585683
C	2.6670702	-3.9125516	2.8465683
O	3.3380702	-2.8915516	2.8485683
C	0.7030702	-4.4145516	1.4085683
C	1.3410702	-3.6995516	0.2315683
C	0.9660702	-4.4035516	-1.0584317
N	-0.4979298	-4.4025516	-1.2224317
C	-1.1359298	-4.7145516	-2.3474317
N	-0.4569298	-5.0465516	-3.4444317
N	-2.4709298	-4.6845516	-2.3574317
N	3.1870702	-5.1275516	2.9065683
C	4.6230702	-5.3055516	2.7465683
C	-0.2569298	-0.6765516	-5.5704317
C	-0.1459298	0.6064484	-5.0134317
C	-0.0259298	0.8094484	-3.6084317
C	-0.0729298	-0.2185516	-2.6484317
I	0.0640702	0.1024484	-0.4934317
C	-0.2309298	-1.4985516	-3.2354317
C	-0.3129298	-1.7215516	-4.6444317
H	5.4651064	-2.1820918	4.4307345
H	3.3516824	-1.1694621	0.3487652
H	5.0940427	-0.9365844	0.1003789
H	2.9378208	1.0570167	-0.8761303
H	4.6793576	1.1756617	-1.1644345
H	2.8694493	-1.0976866	-2.1867434
H	4.6356475	-0.9540280	-2.4724799
H	3.1321095	1.4248508	-3.2559640
H	3.9627528	-1.8671590	-4.2918462
H	3.7290954	-1.5355299	-5.9644235
H	2.8634546	1.8556476	-5.5039352
H	2.9823746	0.5753226	-6.6553870
H	4.9968737	1.1798827	1.4472053
H	0.6702381	2.0083834	2.5502236

H	-2.0988957	3.5166669	-0.8564487
H	-2.2136085	5.1599526	-1.4785614
H	-0.2006422	5.7272719	0.1241104
H	-4.4517097	6.7540192	1.6039624
H	-5.7678667	4.2662018	4.4615008
H	-5.1542607	4.8129484	2.8708843
H	-4.0667609	-0.5073155	0.9423273
H	-5.3728000	0.6972244	0.8859252
H	-3.6106364	2.4665382	0.3195361
H	-2.4201588	1.1926522	0.1891808
H	-4.8990802	1.6863501	-1.5636818
H	-3.1696383	1.7593586	-2.0159901
H	-4.2058222	-0.8554797	-1.1046450
H	-3.5261695	1.2404670	-3.9190360
H	-3.5279557	-0.0708366	-5.0264409
H	-4.4225668	-2.4945902	-2.6176861
H	-4.2579614	-2.1889351	-4.2884112
H	-4.7176415	0.2894199	3.1617512
H	-0.0638889	-0.0143408	3.1336489
H	0.9400744	-5.4913482	1.3791615
H	-0.3984714	-4.3313041	1.4096964
H	2.4390313	-3.7124965	0.3126881
H	1.0378220	-2.6424991	0.1990576
H	1.3286612	-5.4465330	-1.0592442
H	1.4146093	-3.8758645	-1.9196317
H	-1.0459700	-4.0938769	-0.4244535
H	-2.9673403	-4.7280392	-1.4728348
H	-2.9781318	-5.0622355	-3.1507258
H	0.5551848	-5.0562546	-3.4501498
H	-0.9243527	-5.3972725	-4.2724999
H	0.6837199	-4.4173761	3.5606674
H	5.1659689	-5.1127297	3.6863009
H	-0.1475058	1.5100026	-5.6302935
H	0.0083866	1.8804100	-3.3130159
H	-0.2988169	-2.3650130	-2.5790189
H	-0.4214187	-2.7566407	-4.9812496
H	1.5287661	3.3062508	3.4030651
H	-3.5263261	8.1649737	2.2060975
H	-3.5056327	6.6163395	3.1100124
H	-6.9110837	4.4489333	3.1069704
H	4.8328945	-6.3347252	2.4244376
H	4.9991099	-4.5962966	1.9959220
H	7.1970406	-1.6732531	4.3375924
H	6.0422032	-0.7252012	5.2990379
H	-0.3298574	-0.8472654	-6.6471253
H	3.3324212	2.9014467	1.5243434
H	3.9963698	-1.1773798	2.9657186
H	-1.6678502	7.3407366	1.0229121
H	-0.9861517	3.2502413	1.5549965
H	-3.6875215	3.0193639	2.6186448
H	-2.8002492	-1.1785183	3.4264846

H	1.4351801	-1.6797315	2.8189447
H	2.5949377	-5.9365908	3.0521770
H	-0.6320298	-0.4784548	4.7481024

4OC5-two wall receptor

C	6.15607020	-1.32655160	4.38256830
C	5.89807020	-0.42055160	3.16756830
O	6.79707020	0.32844840	2.73656830
N	4.67007020	-0.49455160	2.63656830
C	4.24107020	0.38544840	1.53756830
C	2.89207020	0.93944840	2.04256830
O	2.07807020	0.18244840	2.57556830
C	4.13807020	-0.40255160	0.22756830
C	3.85307020	0.45844840	-1.02043170
C	3.70507020	-0.38155160	-2.30743170
N	3.45407020	0.47644840	-3.45143170
C	3.36507020	0.03644840	-4.71243170
N	3.59907020	-1.24555160	-5.00243170
N	3.09007020	0.88444840	-5.69743170
N	2.69107020	2.24944840	1.97156830
C	1.40007020	2.81344840	2.42456830
C	0.95707020	3.87044840	1.41856830
O	1.76107020	4.69744840	0.99256830
N	-0.33592980	3.87544840	1.07756830
C	-0.95392980	4.94844840	0.29456830
C	-2.15192980	5.36344840	1.11356830
O	-2.94192980	4.52444840	1.52056830
N	-2.34892980	6.65544840	1.32756830
C	-3.52692980	7.07144840	2.10856830
C	-5.88492980	4.16244840	3.37056830
C	-5.67692980	2.68444840	3.01256830
O	-6.62492980	1.87444840	3.09956830
N	-4.41492980	2.31844840	2.77556830
C	-4.07292980	0.92644840	2.53756830
C	-2.57192980	0.79844840	2.90856830
O	-1.86192980	1.79644840	2.85556830
C	-4.28892980	0.57644840	1.06356830
C	-3.49292980	1.39544840	0.09356830
C	-3.91092980	1.22244840	-1.39743170
N	-3.97792980	-0.17755160	-1.82543170
C	-3.90192980	-0.59155160	-3.08543170
N	-4.03792980	-1.90055160	-3.34143170
N	-3.77392980	0.26944840	-4.10343170
N	-2.14592980	-0.42355160	3.23756830
C	-0.75292980	-0.67655160	3.66756830
C	-0.47892980	-2.13955160	3.40656830
O	-1.37192980	-3.01355160	3.61356830
N	0.73207020	-2.42255160	2.93656830
C	1.15707020	-3.82655160	2.75856830
C	2.66707020	-3.91255160	2.84656830
O	3.33807020	-2.89155160	2.84856830

N	3.18707020	-5.12755160	2.90656830
C	4.62307020	-5.30555160	2.74656830
C	-0.25692980	-0.67655160	-5.57043170
C	-0.14592980	0.60644840	-5.01343170
C	-0.02592980	0.80944840	-3.60843170
C	-0.07292980	-0.21855160	-2.64843170
I	0.06407020	0.10244840	-0.49343170
C	-0.23092980	-1.49855160	-3.23543170
C	-0.31292980	-1.72155160	-4.64443170
H	5.46510640	-2.18209180	4.43073450
H	3.35168240	-1.16946210	0.34876520
H	5.09404270	-0.93658440	0.10037890
H	2.93782080	1.05701670	-0.87613030
H	4.67935760	1.17566170	-1.16443450
H	2.86944930	-1.09768660	-2.18674340
H	4.63564750	-0.95402800	-2.47247990
H	3.13210950	1.42485080	-3.25596400
H	3.96275280	-1.86715900	-4.29184620
H	3.72909540	-1.53552990	-5.96442350
H	2.86345460	1.85564760	-5.50393520
H	2.98237460	0.57532260	-6.65538700
H	4.99687370	1.17988270	1.44720530
H	0.67023810	2.00838340	2.55022360
H	-0.20064220	5.72727190	0.12411040
H	-4.45170970	6.75401920	1.60396240
H	-5.76786670	4.26620180	4.46150080
H	-5.15426070	4.81294840	2.87088430
H	-4.06676090	-0.50731550	0.94232730
H	-5.37280000	0.69722440	0.88592520
H	-3.61063640	2.46653820	0.31953610
H	-2.42015880	1.19265220	0.18918080
H	-4.89908020	1.68635010	-1.56368180
H	-3.16963830	1.75935860	-2.01599010
H	-4.20582220	-0.85547970	-1.10464500
H	-3.52616950	1.24046700	-3.91903600
H	-3.52795570	-0.07083660	-5.02644090
H	-4.42256680	-2.49459020	-2.61768610
H	-4.25796140	-2.18893510	-4.28841120
H	-4.71764150	0.28941990	3.16175120
H	-0.06388890	-0.01434080	3.13364890
H	0.68371990	-4.41737610	3.56066740
H	5.16596890	-5.11272970	3.68630090
H	-0.14750580	1.51000260	-5.63029350
H	0.00838660	1.88041000	-3.31301590
H	-0.29881690	-2.36501300	-2.57901890
H	-0.42141870	-2.75664070	-4.98124960
H	1.52876610	3.30625080	3.40306510
H	-3.52632610	8.16497370	2.20609750
H	-3.50563270	6.61633950	3.11001240
H	-6.91108370	4.44893330	3.10697040
H	4.83289450	-6.33472520	2.42443760

H	4.99910990	-4.59629660	1.99592200
H	7.19704060	-1.67325310	4.33759240
H	6.04220320	-0.72520120	5.29903790
H	-0.32985740	-0.84726540	-6.64712530
H	3.33242120	2.90144670	1.52434340
H	3.99636980	-1.17737980	2.96571860
H	-1.66785020	7.34073660	1.02291210
H	-0.98615170	3.25024130	1.55499650
H	-3.68752150	3.01936390	2.61864480
H	-2.80024920	-1.17851830	3.42648460
H	1.43518010	-1.67973150	2.81894470
H	2.59493770	-5.93659080	3.05217700
H	-0.63202980	-0.47845480	4.74810240
H	-1.33891722	4.58626993	-0.63576037
H	0.84181203	-4.23485954	1.82112661

4OC5-no wall receptor

C	6.15607020	-1.32655160	4.38256830
C	5.89807020	-0.42055160	3.16756830
O	6.79707020	0.32844840	2.73656830
N	4.67007020	-0.49455160	2.63656830
C	4.24107020	0.38544840	1.53756830
C	2.89207020	0.93944840	2.04256830
O	2.07807020	0.18244840	2.57556830
N	2.69107020	2.24944840	1.97156830
C	1.40007020	2.81344840	2.42456830
C	0.95707020	3.87044840	1.41856830
O	1.76107020	4.69744840	0.99256830
N	-0.33592980	3.87544840	1.07756830
C	-0.95392980	4.94844840	0.29456830
C	-2.15192980	5.36344840	1.11356830
O	-2.94192980	4.52444840	1.52056830
N	-2.34892980	6.65544840	1.32756830
C	-3.52692980	7.07144840	2.10856830
C	-5.88492980	4.16244840	3.37056830
C	-5.67692980	2.68444840	3.01256830
O	-6.62492980	1.87444840	3.09956830
N	-4.41492980	2.31844840	2.77556830
C	-4.07292980	0.92644840	2.53756830
C	-2.57192980	0.79844840	2.90856830
O	-1.86192980	1.79644840	2.85556830
N	-2.14592980	-0.42355160	3.23756830
C	-0.75292980	-0.67655160	3.66756830
C	-0.47892980	-2.13955160	3.40656830
O	-1.37192980	-3.01355160	3.61356830
N	0.73207020	-2.42255160	2.93656830
C	1.15707020	-3.82655160	2.75856830
C	2.66707020	-3.91255160	2.84656830
O	3.33807020	-2.89155160	2.84856830
N	3.18707020	-5.12755160	2.90656830
C	4.62307020	-5.30555160	2.74656830

C	-0.25692980	-0.67655160	-5.57043170
C	-0.14592980	0.60644840	-5.01343170
C	-0.02592980	0.80944840	-3.60843170
C	-0.07292980	-0.21855160	-2.64843170
I	0.06407020	0.10244840	-0.49343170
C	-0.23092980	-1.49855160	-3.23543170
C	-0.31292980	-1.72155160	-4.64443170
H	5.46510640	-2.18209180	4.43073450
H	4.99687370	1.17988270	1.44720530
H	0.67023810	2.00838340	2.55022360
H	-0.20064220	5.72727190	0.12411040
H	-4.45170970	6.75401920	1.60396240
H	-5.76786670	4.26620180	4.46150080
H	-5.15426070	4.81294840	2.87088430
H	-4.71764150	0.28941990	3.16175120
H	-0.06388890	-0.01434080	3.13364890
H	0.68371990	-4.41737610	3.56066740
H	5.16596890	-5.11272970	3.68630090
H	-0.14750580	1.51000260	-5.63029350
H	0.00838660	1.88041000	-3.31301590
H	-0.29881690	-2.36501300	-2.57901890
H	-0.42141870	-2.75664070	-4.98124960
H	1.52876610	3.30625080	3.40306510
H	-3.52632610	8.16497370	2.20609750
H	-3.50563270	6.61633950	3.11001240
H	-6.91108370	4.44893330	3.10697040
H	4.83289450	-6.33472520	2.42443760
H	4.99910990	-4.59629660	1.99592200
H	7.19704060	-1.67325310	4.33759240
H	6.04220320	-0.72520120	5.29903790
H	-0.32985740	-0.84726540	-6.64712530
H	3.33242120	2.90144670	1.52434340
H	3.99636980	-1.17737980	2.96571860
H	-1.66785020	7.34073660	1.02291210
H	-0.98615170	3.25024130	1.55499650
H	-3.68752150	3.01936390	2.61864480
H	-2.80024920	-1.17851830	3.42648460
H	1.43518010	-1.67973150	2.81894470
H	2.59493770	-5.93659080	3.05217700
H	-0.63202980	-0.47845480	4.74810240
H	-1.33891722	4.58626993	-0.63576037
H	0.84181203	-4.23485954	1.82112661
H	-4.22395856	0.68172587	1.50693684
H	4.16914120	-0.16484340	0.62274310