A novel role for GCR1 in the G-protein-mediated signaling process in plants.

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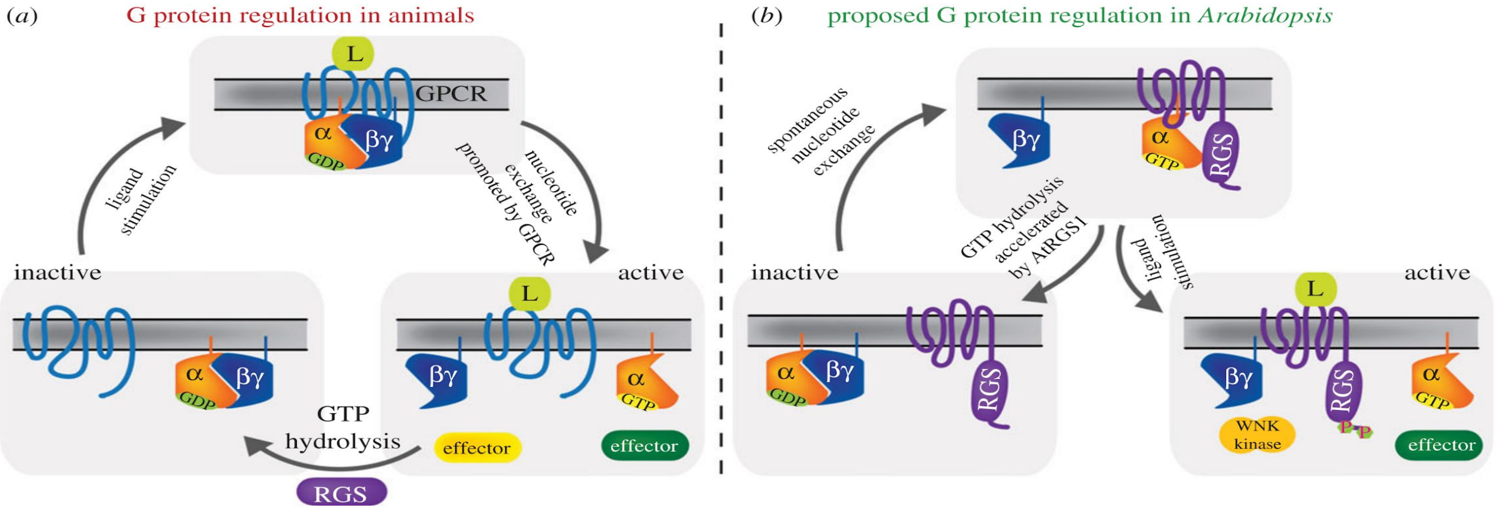
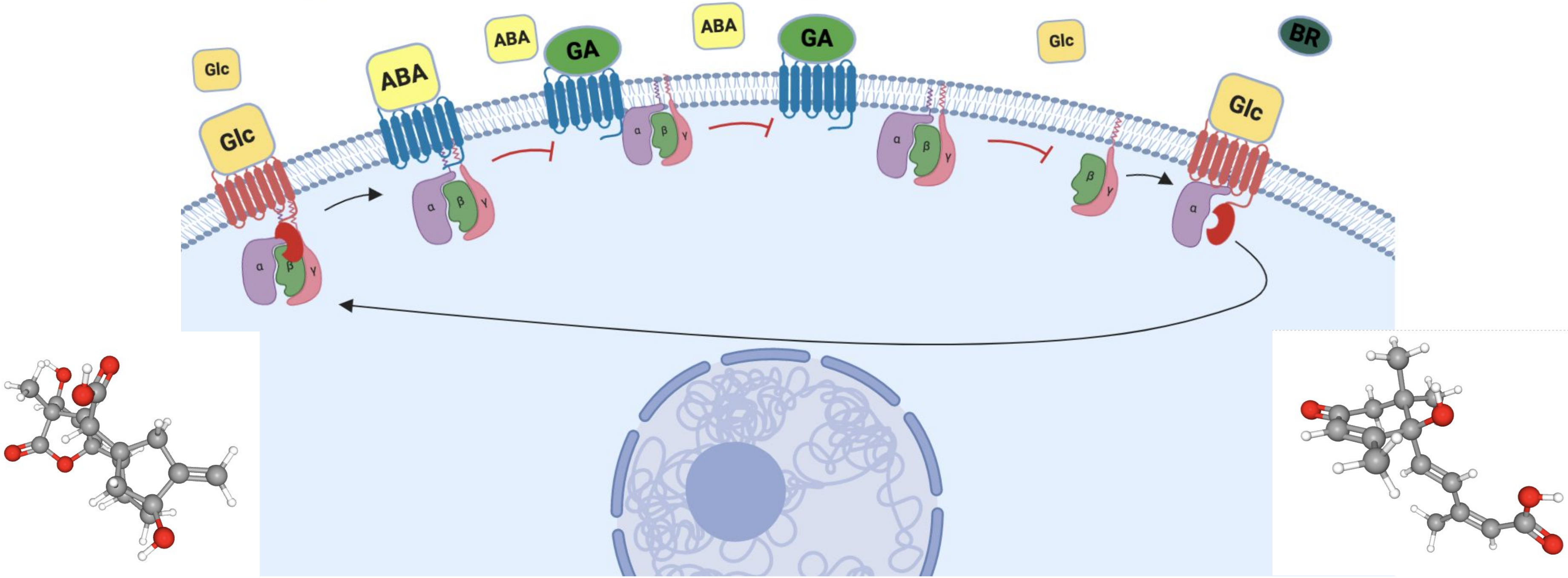
Contrasting Animal and Plant Cell Signaling in Membrane Proteins



GCR1 not required? Urano et al. Open biology. 2013;3: 120186. (image source)
Self-activation of alpha subunit: Johnston et al. 2007. *Proceedings of the National Academy of Sciences of the United States of America,* **104**(44)

Is GCR1 an analog of animal GPCRs? is it needed?

GPCRs can have various active states and bind different kinds of ligands to produce specific responses to each stimulus.



Gibberellin A1

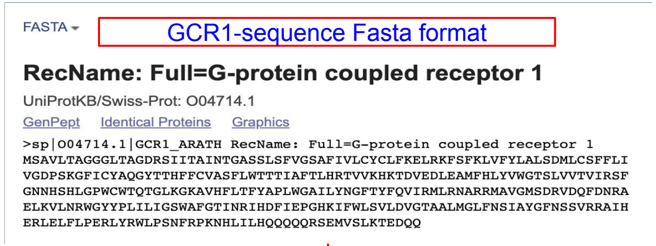
Abscisic Acid

RGS1 has a regulatory GTPase activity on the GTP-Gα subunit. GCR1 would be necessary

Several active states per GPCR: Gray et al. Proceedings of the National Academy of Sciences of the United States of America 2014 Jan 7,;111(1):12.
Evidence of heterotrimer signalling in plants: *Chen et al. PLANT PHYSIOLOGY 2006,* ***141****(3)*
GCR1 internalization: Pandey and Assmann The Plant Cell, , 2004. **16**(6)
CR1 and GPA1 regulate DNA synthesis through PI- PLC activation and IP_3 and DAG production. Apone et al. PLANT PHYSIOLOGY, 2003. **133**(2)

GCR1.mfta file generation

GCR1-sequence Fasta format



RecName: Full=G-protein coupled receptor 1

UniProtKB/Swiss-Prot: O04714.1

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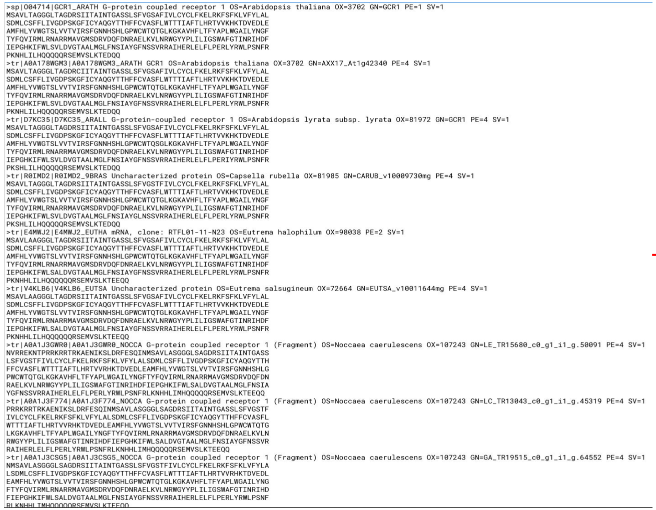
BLAST search



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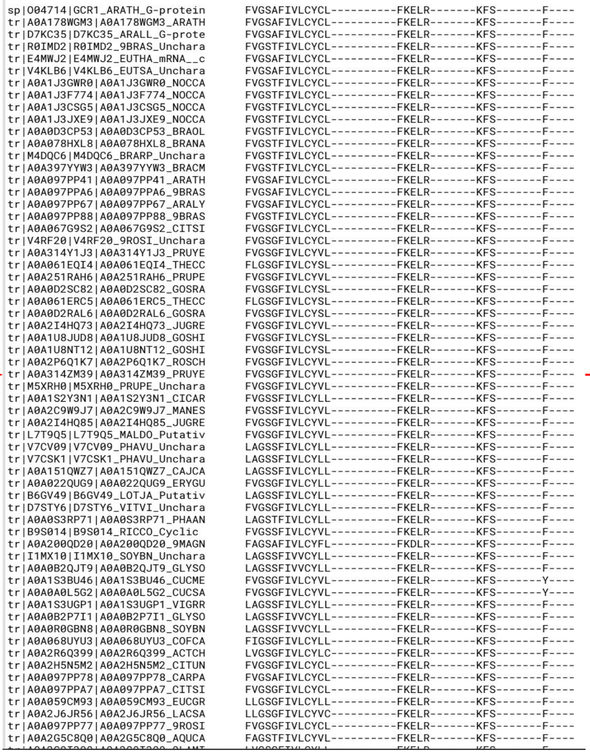
sequence alignment



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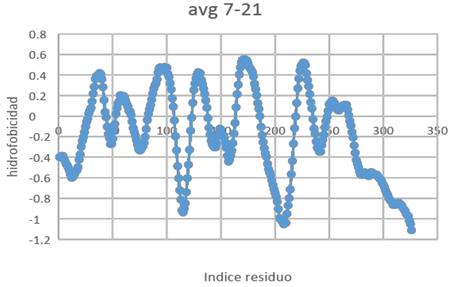
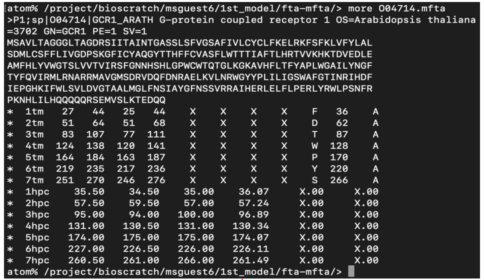
Hydrophobic centers and eta residue



GCR1.mfta



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*  2tm   51   64   51   68    X    X    X    X    D   62    A
*  3tm   83  107   77  111    X    X    X    X    T   87    A
*  4tm  124  138  120  141    X    X    X    X    W  128    A
*  5tm  164  184  163  187    X    X    X    X    P  170    A
*  6tm  219  235  217  236    X    X    X    X    Y  220    A
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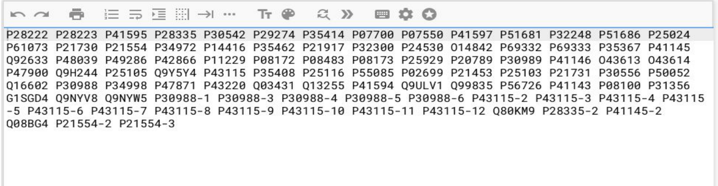
7 TM regions were found up

Condense alignment: GCR1 *Vs* human GPCRs

IDs de GPCRs con estructura 3D def.



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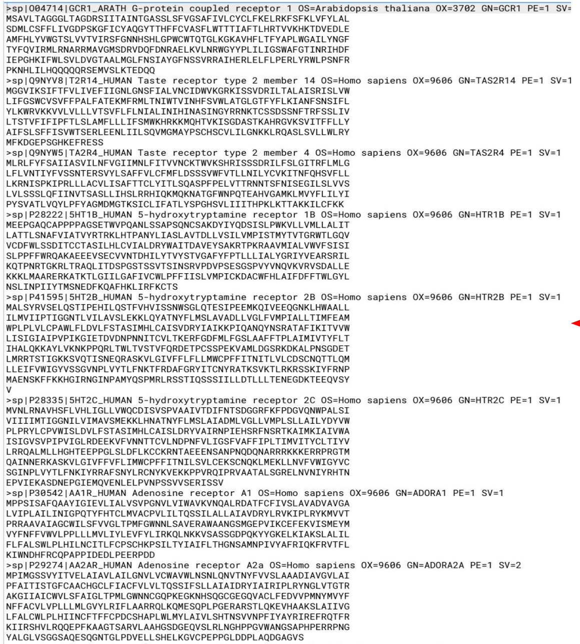
Secuencias de GPCRs con estructura 3D def.



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LIFGSWCVSVFFPALFATEKMFRMLTNIWTVINHFSVWLATGLGTFYFLKIANFSNSIFL
YLKWRVKKVVLVLLLVTSVFLFLNIALINIHINASINGYRRNKTCSSDSSNFTRFSSLIV
LTSTVFIFIPFTLSLAMFLLLIFSMWKHRKKMQHTVKISGDASTKAHRGVKSVITFFLLY
AIFSLSFFISVWTSERLEENLIILSQVMGMAYPSCHSCVLILGNKKLRQASLSVLLWLRY
MFKDGEPSGHKEFRESS
>sp|Q9NYW5|TA2R4_HUMAN Taste receptor type 2 member 4 OS=Homo sapiens OX=9606 GN=TAS2R4 PE=1 SV=1
MLRLFYFSAIIASVILNFVGIIMNLFITVVNCKTWVKSHRISSSDRILFSLGITRFLMLG
LFLVNTIYFVSSNTERSVYLSAFFVLCFMFLDSSSVWFVTLLNILYCVKITNFQHSVFLL
LKRNISPKIPRLLLACVLISAFTTCLYITLSQASPFPELVTTRNNTSFNISEGILSLVVS
LVLSSSLQFIINVTSASLLIHSLRRHIQKMQKNATGFWNPQTEAHVGAMKLMVYFLILYI
PYSVATLVQYLPFYAGMDMGTKSICLIFATLYSPGHSVLIIITHPKLKTTAKKILCFKK
>sp|P28222|5HT1B_HUMAN 5-hydroxytryptamine receptor 1B OS=Homo sapiens OX=9606 GN=HTR1B PE=1 SV=1
MEEPGAQCAPPPPAGSETWVPQANLSSAPSQNCSAKDYIYQDSISLPWKVLLVMLLALIT
LATTLSNAFVIATVYRTRKLHTPANYLIASLAVTDLLVSILVMPISTMYTVTGRWTLGQV
VCDFWLSSDITCCTASILHLCVIALDRYWAITDAVEYSAKRTPKRAAVMIALVWVFSISI
SLPPFFWRQAKAEEEVSECVVNTDHILYTVYSTVGAFYFPTLLLIALYGRIYVEARSRIL
KQTPNRTGKRLTRAQLITDSPGSTSSVTSINSRVPDVPSESGSPVYVNQVKVRVSDALLE
KKKLMAARERKATKTLGIILGAFIVCWLPFFIISLVMPICKDACWFHLAIFDFFTWLGYL
NSLINPIIYTMSNEDFKQAFHKLIRFKCTS
>sp|P41595|5HT2B_HUMAN 5-hydroxytryptamine receptor 2B OS=Homo sapiens OX=9606 GN=HTR2B PE=1 SV=1
MALSYRVSELQSTIPEHILQSTFVHVISSNWSGLQTESIPEEMKQIVEEQGNKLHWAALL
ILMVIIPTIGGNTLVILAVSLEKKLQYATNYFLMSLAVADLLVGLFVMPIALLTIMFEAM
WPLPLVLCPAWLFLDVLFSTASIMHLCAISVDRYIAIKKPIQANQYNSRATAFIKITVVW
LISIGIAIPVPIKGIETDVDNPNNITCVLTKERFGDFMLFGSLAAFFTPLAIMIVTYFLT
IHALQKKAYLVKNKPPQRLTWLTVSTVFQRDETPCSSPEKVAMLDGSRKDKALPNSGDET
LMRRTSTIGKKSVQTISNEQRASKVLGIVFFLFLLMWCPFFITNITLVLCDSCNQTTLQM
LLEIFVWIGYVSSGVNPLVYTLFNKTFRDAFGRYITCNYRATKSVKTLRKRSSKIYFRNP
MAENSKFFKKHGIRNGINPAMYQSPMRLRSSTIQSSSIILLDTLLLTENEGDKTEEQVSY
V
>sp|P28335|5HT2C_HUMAN 5-hydroxytryptamine receptor 2C OS=Homo sapiens OX=9606 GN=HTR2C PE=1 SV=1
MVNLRNAVHSFLVHLIGLLVWQCDISVSPVAAIVTDIFNTSDGGRFKFPDGVQNWPALSI
VIIIIMTIGGNILVIMAVSMEKKLHNATNYFLMSLAIADMLVGLLVMPLSLLAILYDYVW
PLPRYLCPVWISLDVLFSTASIMHLCAISLDRYVAIRNPIEHSRFNSRTKAIMKIAIVWA
ISIGVSVPIPVIGLRDEEKVFVNNTTCVLNDPNFVLIGSFVAFFIPLTIMVITYCLTIYV
LRRQALMLLHGHTEEPPGLSLDFLKCCKRNTAEEENSANPNQDQNARRRKKKERRPRGTM
QAINNERKASKVLGIVFFVFLIMWCPFFITNILSVLCEKSCNQKLMEKLLNVFVWIGYVC
SGINPLVYTLFNKIYRRAFSNYLRCNYKVEKKPPVRQIPRVAATALSGRELNVNIYRHTN
EPVIEKASDNEPGIEMQVENLELPVNPSSVVSERISSV
>sp|P30542|AA1R_HUMAN Adenosine receptor A1 OS=Homo sapiens OX=9606 GN=ADORA1 PE=1 SV=1
MPPSISAFQAAYIGIEVLIALVSVPGNVLVIWAVKVNQALRDATFCFIVSLAVADVAVGA
LVIPLAILINIGPQTYFHTCLMVACPVLILTQSSILALLAIAVDRYLRVKIPLRYKMVVT
PRRAAVAIAGCWILSFVVGLTPMFGWNNLSAVERAWAANGSMGEPVIKCEFEKVISMEYM
VYFNFFVWVLPPLLLMVLIYLEVFYLIRKQLNKKVSASSGDPQKYYGKELKIAKSLALIL
FLFALSWLPLHILNCITLFCPSCHKPSILTYIAIFLTHGNSAMNPIVYAFRIQKFRVTFL
KIWNDHFRCQPAPPIDEDLPEERPDD
>sp|P29274|AA2AR_HUMAN Adenosine receptor A2a OS=Homo sapiens OX=9606 GN=ADORA2A PE=1 SV=2
MPIMGSSVYITVELAIAVLAILGNVLVCWAVWLNSNLQNVTNYFVVSLAAADIAVGVLAI
PFAITISTGFCAACHGCLFIACFVLVLTQSSIFSLLAIAIDRYIAIRIPLRYNGLVTGTR
AKGIIAICWVLSFAIGLTPMLGWNNCGQPKEGKNHSQGCGEGQVACLFEDVVPMNYMVYF
NFFACVLVPLLLMLGVYLRIFLAARRQLKQMESQPLPGERARSTLQKEVHAAKSLAIIVG
LFALCWLPLHIINCFTFFCPDCSHAPLWLMYLAIVLSHTNSVVNPFIYAYRIREFRQTFR
KIIRSHVLRQQEPFKAAGTSARVLAAHGSDGEQVSLRLNGHPPGVWANGSAPHPERRPNG
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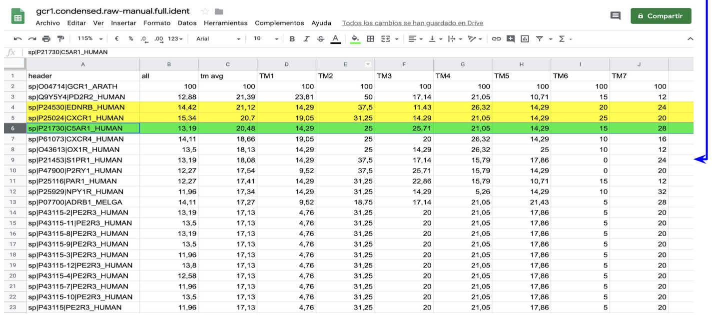
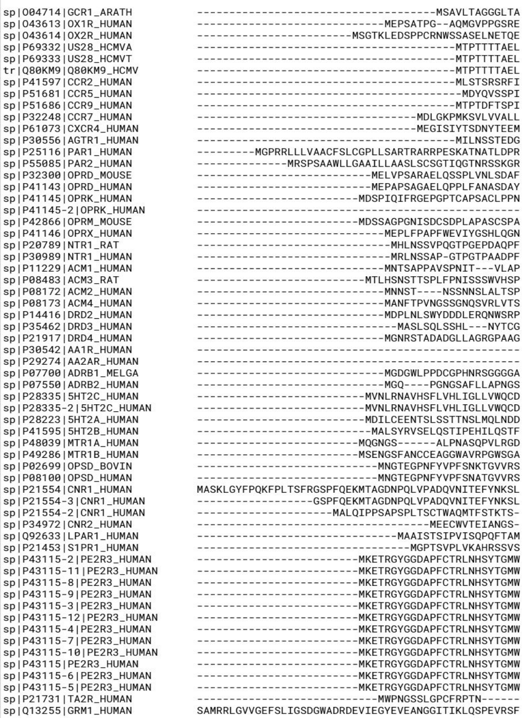


	A	B	C	D	E	F	G	H	I	J
1	header	all	tm avg	TM1	TM2	TM3	TM4	TM5	TM6	TM7
2	sp|O04714|GCR1_ARATH	100	100	100	100	100	100	100	100	100
3	sp|Q9Y5Y4|PD2R2_HUMAN	12,88	21,39	23,81	50	17,14	21,05	10,71	15	12
4	sp|P24530|EDNRB_HUMAN	14,42	21,12	14,29	37,5	11,43	26,32	14,29	20	24
5	sp|P25024|CXCR1_HUMAN	15,34	20,7	19,05	31,25	14,29	21,05	14,29	25	20
6	sp|P21730|C5AR1_HUMAN	13,19	20,48	14,29	25	25,71	21,05	14,29	15	28
7	sp|P61073|CXCR4_HUMAN	14,11	18,66	19,05	25	20	26,32	14,29	10	16
8	sp|O43613|OX1R_HUMAN	13,5	18,13	14,29	25	14,29	26,32	25	10	12
9	sp|P21453|S1PR1_HUMAN	13,19	18,08	14,29	37,5	17,14	15,79	17,86	0	24
10	sp|P47900|P2RY1_HUMAN	12,27	17,54	9,52	37,5	25,71	15,79	14,29	0	20
11	sp|P25116|PAR1_HUMAN	12,27	17,41	14,29	31,25	22,86	15,79	10,71	15	12
12	sp|P25929|NPY1R_HUMAN	11,96	17,34	14,29	31,25	14,29	5,26	14,29	10	32
13	sp|P07700|ADRB1_MELGA	14,11	17,27	9,52	18,75	17,14	21,05	21,43	5	28
14	sp|P43115-2|PE2R3_HUMAN	13,19	17,13	4,76	31,25	20	21,05	17,86	5	20
15	sp|P43115-11|PE2R3_HUMAN	13,5	17,13	4,76	31,25	20	21,05	17,86	5	20
16	sp|P43115-8|PE2R3_HUMAN	13,19	17,13	4,76	31,25	20	21,05	17,86	5	20
17	sp|P43115-9|PE2R3_HUMAN	13,5	17,13	4,76	31,25	20	21,05	17,86	5	20
18	sp|P43115-3|PE2R3_HUMAN	11,96	17,13	4,76	31,25	20	21,05	17,86	5	20
19	sp|P43115-12|PE2R3_HUMAN	13,8	17,13	4,76	31,25	20	21,05	17,86	5	20
20	sp|P43115-4|PE2R3_HUMAN	12,58	17,13	4,76	31,25	20	21,05	17,86	5	20
21	sp|P43115-7|PE2R3_HUMAN	11,96	17,13	4,76	31,25	20	21,05	17,86	5	20
22	sp|P43115-10|PE2R3_HUMAN	13,5	17,13	4,76	31,25	20	21,05	17,86	5	20
23	sp|P43115|PE2R3_HUMAN	11,96	17,13	4,76	31,25	20	21,05	17,86	5	20

Alineamiento secuencias



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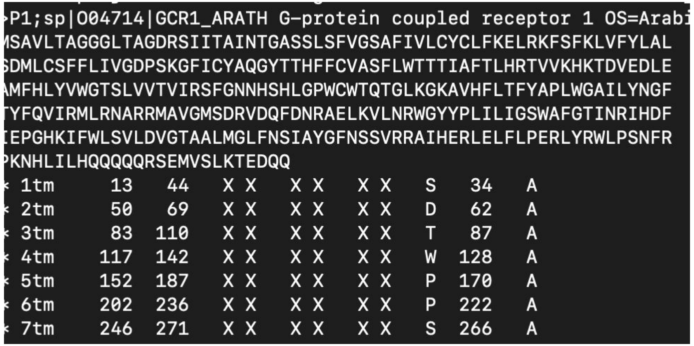
sp|O04714|GCR1_ARATH          -------------------------------------MSAVLTAGGGLTA
sp|O43613|OX1R_HUMAN          -----------------------------MEPSATPG--AQMGVPPGSRE
sp|O43614|OX2R_HUMAN          ------------------------MSGTKLEDSPPCRNWSSASELNETQE
sp|P69332|US28_HCMVA          ----------------------------------------MTPTTTTAEL
sp|P69333|US28_HCMVT          ----------------------------------------MTPTTTTAEL
tr|Q80KM9|Q80KM9_HCMV         ----------------------------------------MTPTTTTAEL
sp|P41597|CCR2_HUMAN          ----------------------------------------MLSTSRSRFI
sp|P51681|CCR5_HUMAN          -----------------------------------------MDYQVSSPI
sp|P51686|CCR9_HUMAN          ----------------------------------------MTPTDFTSPI
sp|P32248|CCR7_HUMAN          ----------------------------------MDLGKPMKSVLVVALL
sp|P61073|CXCR4_HUMAN         ----------------------------------MEGISIYTSDNYTEEM
sp|P30556|AGTR1_HUMAN         ----------------------------------------MILNSSTEDG
sp|P25116|PAR1_HUMAN          ---------MGPRRLLLVAACFSLCGPLLSARTRARRPESKATNATLDPR
sp|P55085|PAR2_HUMAN          --------------MRSPSAAWLLGAAILLAASLSCSGTIQGTNRSSKGR
sp|P32300|OPRD_MOUSE          ---------------------------MELVPSARAELQSSPLVNLSDAF
sp|P41143|OPRD_HUMAN          ---------------------------MEPAPSAGAELQPPLFANASDAY
sp|P41145|OPRK_HUMAN          -------------------------MDSPIQIFRGEPGPTCAPSACLPPN
sp|P41145-2|OPRK_HUMAN        --------------------------------------------------
sp|P42866|OPRM_MOUSE          -------------------------MDSSAGPGNISDCSDPLAPASCSPA
sp|P41146|OPRX_HUMAN          -----------------------------MEPLFPAPFWEVIYGSHLQGN
sp|P20789|NTR1_RAT            ------------------------------MHLNSSVPQGTPGEPDAQPF
sp|P30989|NTR1_HUMAN          ------------------------------MRLNSSAP-GTPGTPAADPF
sp|P11229|ACM1_HUMAN          -----------------------------MNTSAPPAVSPNIT---VLAP
sp|P08483|ACM3_RAT            --------------------------MTLHSNSTTSPLFPNISSSWVHSP
sp|P08172|ACM2_HUMAN          -----------------------------MNNST----NSSNNSLALTSP
sp|P08173|ACM4_HUMAN          -----------------------------MANFTPVNGSSGNQSVRLVTS
sp|P14416|DRD2_HUMAN          -----------------------------MDPLNLSWYDDDLERQNWSRP
sp|P35462|DRD3_HUMAN          -------------------------------MASLSQLSSHL---NYTCG
sp|P21917|DRD4_HUMAN          -----------------------------MGNRSTADADGLLAGRGPAAG
sp|P30542|AA1R_HUMAN          --------------------------------------------------
sp|P29274|AA2AR_HUMAN         --------------------------------------------------
sp|P07700|ADRB1_MELGA         -----------------------------MGDGWLPPDCGPHNRSGGGGA
sp|P07550|ADRB2_HUMAN         -----------------------------MGQ----PGNGSAFLLAPNGS
sp|P28335|5HT2C_HUMAN         --------------------------MVNLRNAVHSFLVHLIGLLVWQCD
sp|P28335-2|5HT2C_HUMAN       --------------------------MVNLRNAVHSFLVHLIGLLVWQCD
sp|P28223|5HT2A_HUMAN         --------------------------MDILCEENTSLSSTTNSLMQLNDD
sp|P41595|5HT2B_HUMAN         ---------------------------MALSYRVSELQSTIPEHILQSTF
sp|P48039|MTR1A_HUMAN         -------------------------MQGNGS------ALPNASQPVLRGD
sp|P49286|MTR1B_HUMAN         -------------------------MSENGSFANCCEAGGWAVRPGWSGA
sp|P02699|OPSD_BOVIN          ----------------------------MNGTEGPNFYVPFSNKTGVVRS
sp|P08100|OPSD_HUMAN          ----------------------------MNGTEGPNFYVPFSNATGVVRS
sp|P21554|CNR1_HUMAN          MASKLGYFPQKFPLTSFRGSPFQEKMTAGDNPQLVPADQVNITEFYNKSL
sp|P21554-3|CNR1_HUMAN        ------------------GSPFQEKMTAGDNPQLVPADQVNITEFYNKSL
sp|P21554-2|CNR1_HUMAN        ---------------------MALQIPPSAPSPLTSCTWAQMTFSTKTS-
sp|P34972|CNR2_HUMAN          ------------------------------------MEECWVTEIANGS-
sp|Q92633|LPAR1_HUMAN         -------------------------------MAAISTSIPVISQPQFTAM
sp|P21453|S1PR1_HUMAN         ---------------------------------MGPTSVPLVKAHRSSVS
sp|P43115-2|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-11|PE2R3_HUMAN      -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-8|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-9|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-3|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-12|PE2R3_HUMAN      -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-4|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-7|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-10|PE2R3_HUMAN      -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115|PE2R3_HUMAN         -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-6|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P43115-5|PE2R3_HUMAN       -------------------------MKETRGYGGDAPFCTRLNHSYTGMW
sp|P21731|TA2R_HUMAN          ----------------------------MWPNGSSLGPCFRPTN------
sp|Q13255|GRM1_HUMAN          SAMRRLGVVGEFSLIGSDGWADRDEVIEGYEVEANGGITIKLQSPEVRSF
```

Homology procedure based on sequence alignment

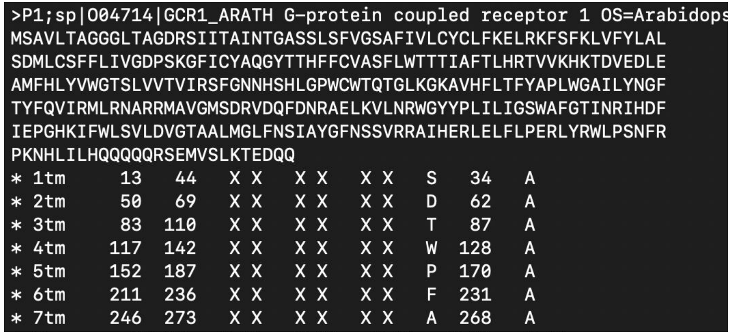
GCR1.mfta

Model 1

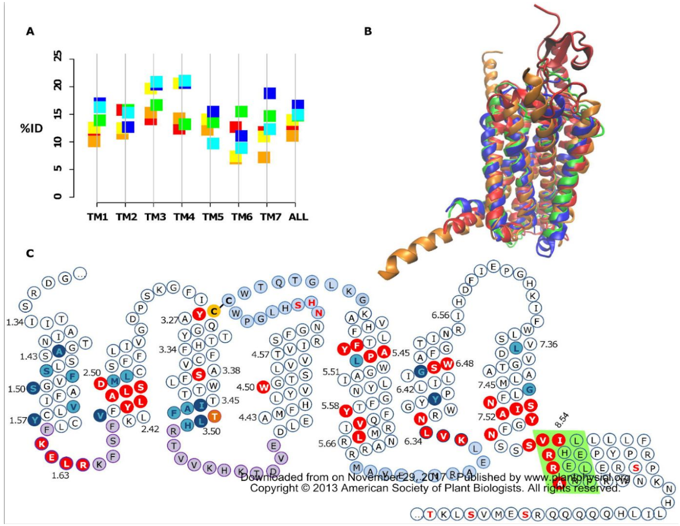


```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabi
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm     13   44   X X   X X   X X   S   34   A
* 2tm     50   69   X X   X X   X X   D   62   A
* 3tm     83  110   X X   X X   X X   T   87   A
* 4tm    117  142   X X   X X   X X   W  128   A
* 5tm    152  187   X X   X X   X X   P  170   A
* 6tm    202  236   X X   X X   X X   P  222   A
* 7tm    246  271   X X   X X   X X   S  266   A
```

Model 2



```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidops
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm     13   44   X X   X X   X X   S   34   A
* 2tm     50   69   X X   X X   X X   D   62   A
* 3tm     83  110   X X   X X   X X   T   87   A
* 4tm    117  142   X X   X X   X X   W  128   A
* 5tm    152  187   X X   X X   X X   P  170   A
* 6tm    211  236   X X   X X   X X   F  231   A
* 7tm    246  273   X X   X X   X X   A  268   A
```

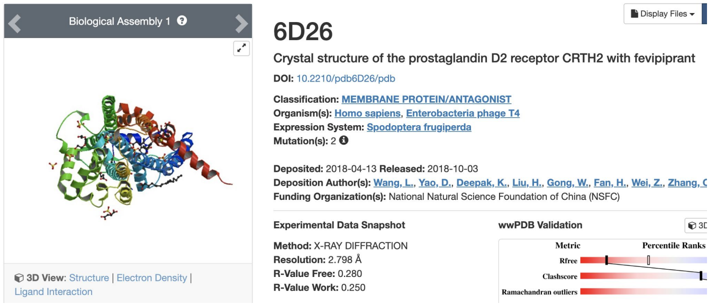


Model 3

```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidop
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
*  1tm   27   44   25   44    X    X    X    X    F   36    A
*  2tm   51   64   51   68    X    X    X    X    D   62    A
*  3tm   83  107   77  111    X    X    X    X    T   87    A
*  4tm  124  138  120  141    X    X    X    X    W  128    A
*  5tm  164  184  163  187    X    X    X    X    P  170    A
*  6tm  219  235  217  236    X    X    X    X    Y  220    A
*  7tm  251  270  246  276    X    X    X    X    S  266    A
```

GCR1 3D structure by homology: Vohra S, Taddese B, Conner AC, Poyner DR, Hay DL, Barwell J, et al. Research. Research. 2013.

Selected templates



6D26

Crystal structure of the prostaglandin D2 receptor CRTH2 with fevipiprant

DOI: 10.2210/pdb6D26/pdb

Classification: MEMBRANE PROTEIN/ANTAGONIST
Organism(s): Homo sapiens, Enterobacteria phage T4
Expression System: Spodoptera frugiperda
Mutation(s): 2

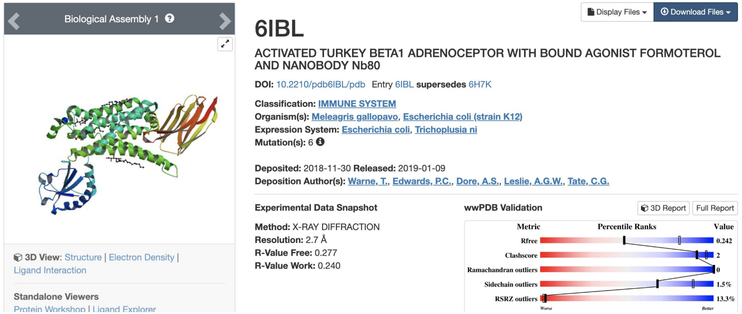
Deposited: 2018-04-13 **Released:** 2018-10-03
Deposition Author(s): Wang, L., Yao, D., Deepak, K., Liu, H., Gong, W., Fan, H., Wei, Z., Zhang, C
Funding Organization(s): National Natural Science Foundation of China (NSFC)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.798 Å
R-Value Free: 0.280
R-Value Work: 0.250

wwPDB Validation

3D View: Structure | Electron Density | Ligand Interaction



6IBL

ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND AGONIST FORMOTEROL AND NANOBODY Nb80

DOI: 10.2210/pdb6IBL/pdb Entry 6IBL **supersedes** 6H7K

Classification: IMMUNE SYSTEM
Organism(s): Meleagris gallopavo, Escherichia coli (strain K12)
Expression System: Escherichia coli, Trichoplusia ni
Mutation(s): 6

Deposited: 2018-11-30 **Released:** 2019-01-09
Deposition Author(s): Warne, T., Edwards, P.C., Dore, A.S., Leslie, A.G.W., Tate, C.G.

Experimental Data Snapshot

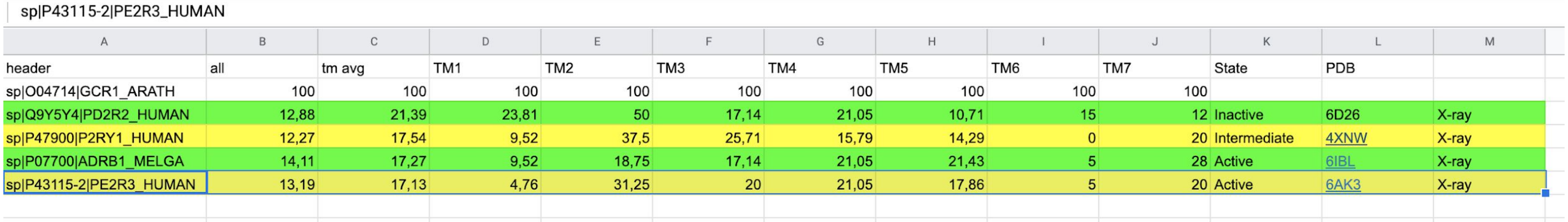
Method: X-RAY DIFFRACTION
Resolution: 2.7 Å
R-Value Free: 0.277
R-Value Work: 0.240

wwPDB Validation

Metric	Value
Rfree	0.242
Clashscore	2
Ramachandran outliers	0
Sidechain outliers	1.5%
RSRZ outliers	13.3%

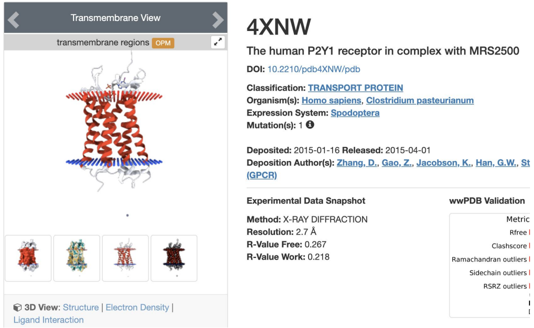
3D View: Structure | Electron Density | Ligand Interaction

Standalone Viewers
Protein Workshop | Ligand Explorer



sp|P43115-2|PE2R3_HUMAN

header	all	tm avg	TM1	TM2	TM3	TM4	TM5	TM6	TM7	State	PDB	
sp|O04714|GCR1_ARATH	100	100	100	100	100	100	100	100	100			
sp|Q9Y5Y4|PD2R2_HUMAN	12,88	21,39	23,81	50	17,14	21,05	10,71	15	12	Inactive	6D26	X-ray
sp|P47900|P2RY1_HUMAN	12,27	17,54	9,52	37,5	25,71	15,79	14,29	0	20	Intermediate	4XNW	X-ray
sp|P07700|ADRB1_MELGA	14,11	17,27	9,52	18,75	17,14	21,05	21,43	5	28	Active	6IBL	X-ray
sp|P43115-2|PE2R3_HUMAN	13,19	17,13	4,76	31,25	20	21,05	17,86	5	20	Active	6AK3	X-ray



4XNW

The human P2Y1 receptor in complex with MRS2500

DOI: 10.2210/pdb4XNW/pdb

Classification: TRANSPORT PROTEIN
Organism(s): Homo sapiens, Clostridium pasteurianum
Expression System: Spodoptera
Mutation(s): 1

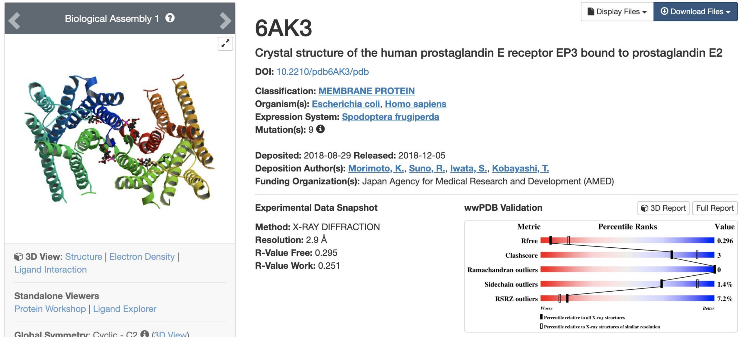
Deposited: 2015-01-16 **Released:** 2015-04-01
Deposition Author(s): Zhang, D., Gao, Z., Jacobson, K., Han, G.W., St
(GPCR)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.7 Å
R-Value Free: 0.267
R-Value Work: 0.218

wwPDB Validation

3D View: Structure | Electron Density | Ligand Interaction



6AK3

Crystal structure of the human prostaglandin E receptor EP3 bound to prostaglandin E2

DOI: 10.2210/pdb6AK3/pdb

Classification: MEMBRANE PROTEIN
Organism(s): Escherichia coli, Homo sapiens
Expression System: Spodoptera frugiperda
Mutation(s): 9

Deposited: 2018-08-29 **Released:** 2018-12-05
Deposition Author(s): Morimoto, K., Suno, R., Iwata, S., Kobayashi, T.
Funding Organization(s): Japan Agency for Medical Research and Development (AMED)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.9 Å
R-Value Free: 0.295
R-Value Work: 0.251

wwPDB Validation

Metric	Value
Rfree	0.296
Clashscore	3
Ramachandran outliers	0
Sidechain outliers	1.4%
RSRZ outliers	7.2%

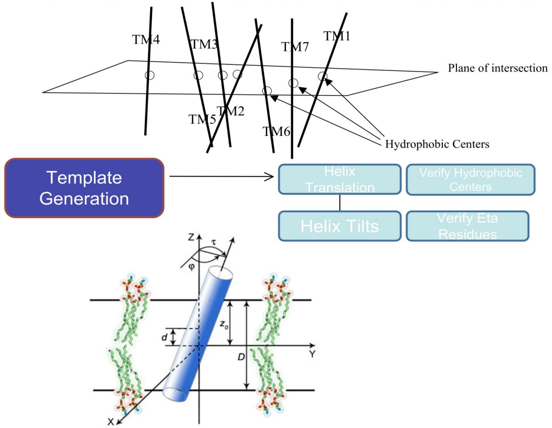
3D View: Structure | Electron Density | Ligand Interaction

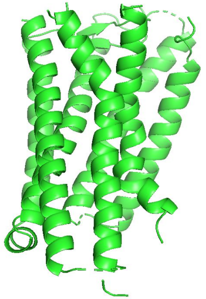
Standalone Viewers
Protein Workshop | Ligand Explorer

Global Symmetry: Cyclic - C2 (3D View)

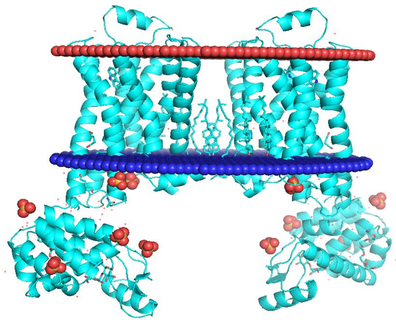
Condense alignment

PE2R3 (Human prostaglandin E receptor EP3.)

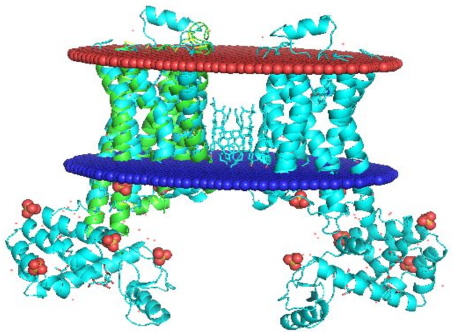


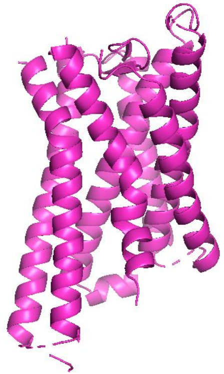


6ak3_chainB.pdb



hBeta2_2rh1_opm.pdb



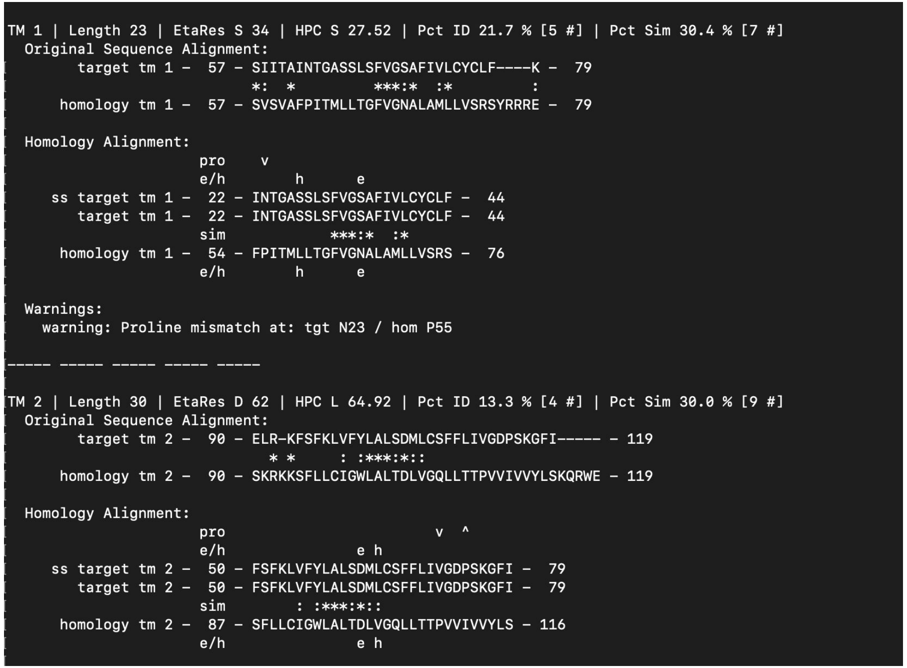


6ak3_chainB_align.pdb

PE2R3.bgf and PE2R3.mfa files

Scott, Caitlin E. Biogroup Methods GPCR Structure Prediction. 2010

Homologize Procedure: target and templates.



```
TM 1 | Length 23 | EtaRes S 34 | HPC S 27.52 | Pct ID 21.7 % [5 #] | Pct Sim 30.4 % [7 #]
  Original Sequence Alignment:
        target tm 1 -  57 - SIITAINTGASSLSFVGSAFIVLCYCLF----K -  79
                            *:  *         ***:*  :*         :
      homology tm 1 -  57 - SVSVAFPITMLLTGFVGNALAMLLVSRSYRRRE -  79

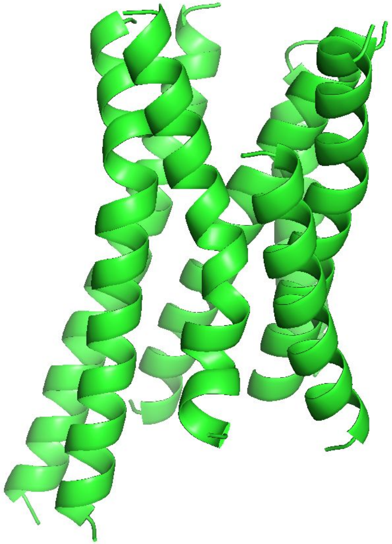
  Homology Alignment:
                      pro    v
                      e/h        h      e
     ss target tm 1 -  22 - INTGASSLSFVGSAFIVLCYCLF -  44
        target tm 1 -  22 - INTGASSLSFVGSAFIVLCYCLF -  44
                      sim            ***:*  :*
      homology tm 1 -  54 - FPITMLLTGFVGNALAMLLVSRS -  76
                      e/h        h      e

  Warnings:
    warning: Proline mismatch at: tgt N23 / hom P55

----- ----- ----- ----- -----

TM 2 | Length 30 | EtaRes D 62 | HPC L 64.92 | Pct ID 13.3 % [4 #] | Pct Sim 30.0 % [9 #]
  Original Sequence Alignment:
        target tm 2 -  90 - ELR-KFSFKLVFYLALSDMLCSFFLIVGDPSKGFI----- - 119
                              * *     : :***:*::
      homology tm 2 -  90 - SKRKKSFLLCIGWLALTDLVGQLLTTPVVIVVYLSKQRWE - 119

  Homology Alignment:
                      pro                        v  ^
                      e/h               e h
     ss target tm 2 -  50 - FSFKLVFYLALSDMLCSFFLIVGDPSKGFI -  79
        target tm 2 -  50 - FSFKLVFYLALSDMLCSFFLIVGDPSKGFI -  79
                      sim        : :***:*::
      homology tm 2 -  87 - SFLLCIGWLALTDLVGQLLTTPVVIVVYLS - 116
                      e/h               e h
```

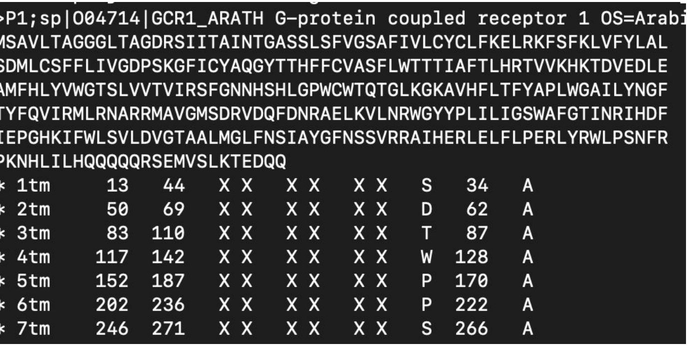


GCR1_PE2R3.PE2R3.hom.bgf

GCR1_PE2R3.bgf from homology

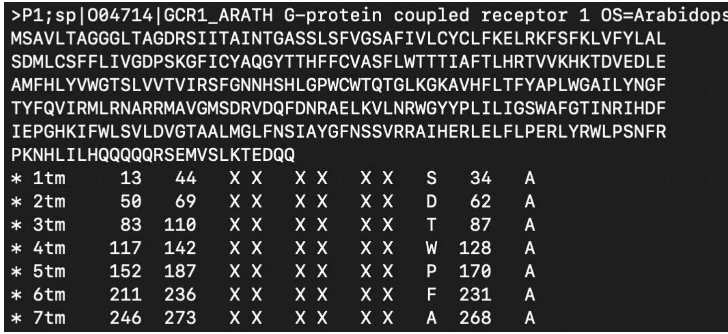
BiHelix

Model 1



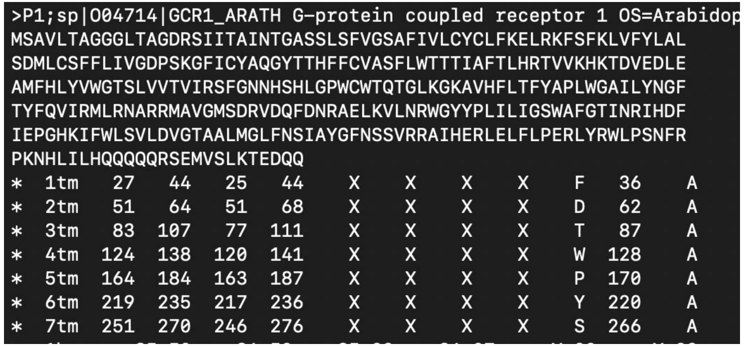
```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabi
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm      13   44   X X   X X   X X   S   34   A
* 2tm      50   69   X X   X X   X X   D   62   A
* 3tm      83  110   X X   X X   X X   T   87   A
* 4tm     117  142   X X   X X   X X   W  128   A
* 5tm     152  187   X X   X X   X X   P  170   A
* 6tm     202  236   X X   X X   X X   P  222   A
* 7tm     246  271   X X   X X   X X   S  266   A
```

Model 2

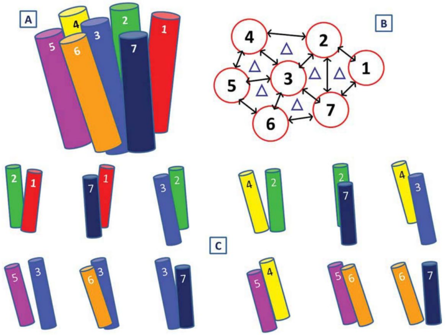


```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidops
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm      13   44   X X   X X   X X   S   34   A
* 2tm      50   69   X X   X X   X X   D   62   A
* 3tm      83  110   X X   X X   X X   T   87   A
* 4tm     117  142   X X   X X   X X   W  128   A
* 5tm     152  187   X X   X X   X X   P  170   A
* 6tm     211  236   X X   X X   X X   F  231   A
* 7tm     246  273   X X   X X   X X   A  268   A
```

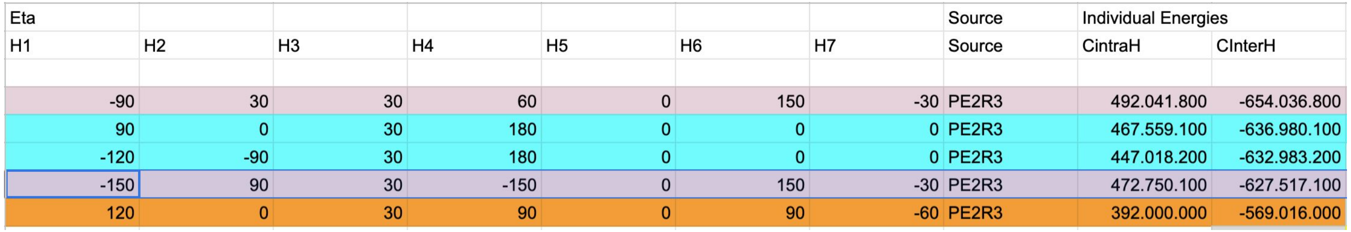
Model 3



```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidop
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
*  1tm   27   44   25   44     X    X    X    X    F   36    A
*  2tm   51   64   51   68     X    X    X    X    D   62    A
*  3tm   83  107   77  111     X    X    X    X    T   87    A
*  4tm  124  138  120  141     X    X    X    X    W  128    A
*  5tm  164  184  163  187     X    X    X    X    P  170    A
*  6tm  219  235  217  236     X    X    X    X    Y  220    A
*  7tm  251  270  246  276     X    X    X    X    S  266    A
```



GCR1.mfta

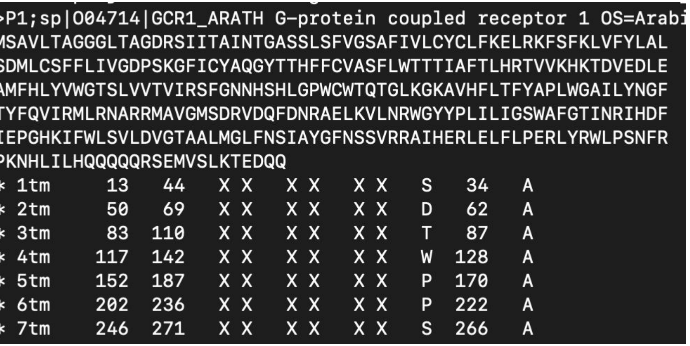


Eta							Source	Individual Energies	
H1	H2	H3	H4	H5	H6	H7	Source	CintraH	CInterH
-90	30	30	60	0	150	-30	PE2R3	492.041.800	-654.036.800
90	0	30	180	0	0	0	PE2R3	467.559.100	-636.980.100
-120	-90	30	180	0	0	0	PE2R3	447.018.200	-632.983.200
-150	90	30	-150	0	150	-30	PE2R3	472.750.100	-627.517.100
120	0	30	90	0	90	-60	PE2R3	392.000.000	-569.016.000

Bray, J. K.; Abrol, R.; Goddard, W. A.; et al. Proceedings of the National Academy of Sciences. 2014

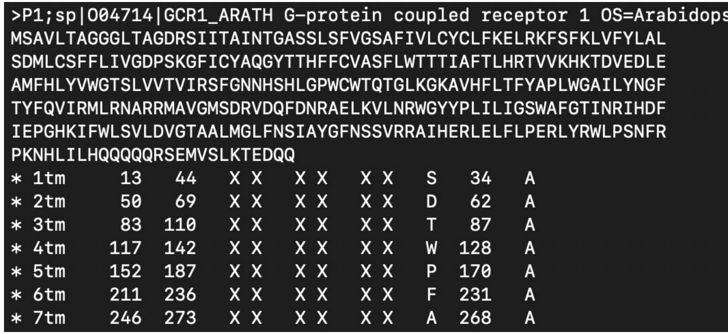
BiHelix

Model 1



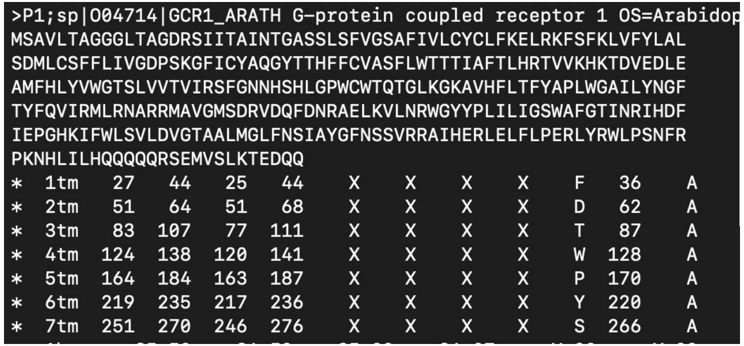
```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabi
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm     13   44   X X   X X   X X   S   34   A
* 2tm     50   69   X X   X X   X X   D   62   A
* 3tm     83  110   X X   X X   X X   T   87   A
* 4tm    117  142   X X   X X   X X   W  128   A
* 5tm    152  187   X X   X X   X X   P  170   A
* 6tm    202  236   X X   X X   X X   P  222   A
* 7tm    246  271   X X   X X   X X   S  266   A
```

Model 2

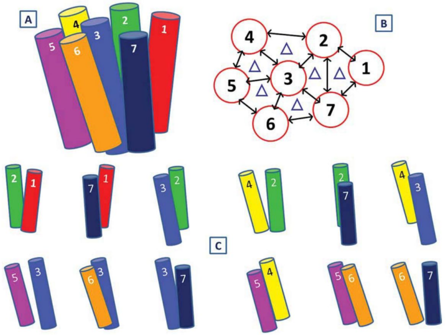


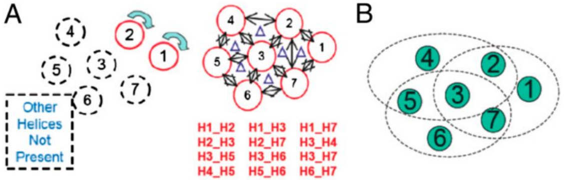
```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidops
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm     13   44   X X   X X   X X   S   34   A
* 2tm     50   69   X X   X X   X X   D   62   A
* 3tm     83  110   X X   X X   X X   T   87   A
* 4tm    117  142   X X   X X   X X   W  128   A
* 5tm    152  187   X X   X X   X X   P  170   A
* 6tm    211  236   X X   X X   X X   F  231   A
* 7tm    246  273   X X   X X   X X   A  268   A
```

Model 3

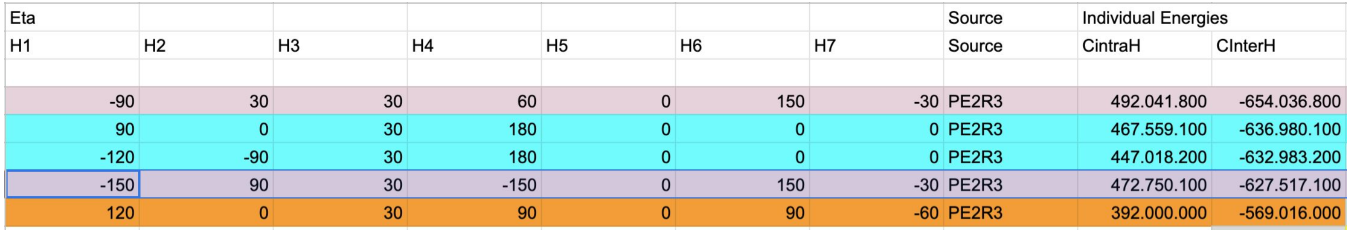


```
>P1;sp|O04714|GCR1_ARATH G-protein coupled receptor 1 OS=Arabidop
MSAVLTAGGGLTAGDRSIITAINTGASSLSFVGSAFIVLCYCLFKELRKFSFKLVFYLAL
SDMLCSFFLIVGDPSKGFICYAQGYTTHFFCVASFLWTTTIAFTLHRTVVKHKTDVEDLE
AMFHLYVWGTSLVVTVIRSFGNNHSHLGPWCWTQTGLKGKAVHFLTFYAPLWGAILYNGF
TYFQVIRMLRNARRMAVGMSDRVDQFDNRAELKVLNRWGYYPLILIGSWAFGTINRIHDF
IEPGHKIFWLSVLDVGTAALMGLFNSIAYGFNSSVRRAIHERLELFLPERLYRWLPSNFR
PKNHLILHQQQQQRSEMVSLKTEDQQ
* 1tm   27   44   25   44   X   X   X   X   F   36   A
* 2tm   51   64   51   68   X   X   X   X   D   62   A
* 3tm   83  107   77  111   X   X   X   X   T   87   A
* 4tm  124  138  120  141   X   X   X   X   W  128   A
* 5tm  164  184  163  187   X   X   X   X   P  170   A
* 6tm  219  235  217  236   X   X   X   X   Y  220   A
* 7tm  251  270  246  276   X   X   X   X   S  266   A
```





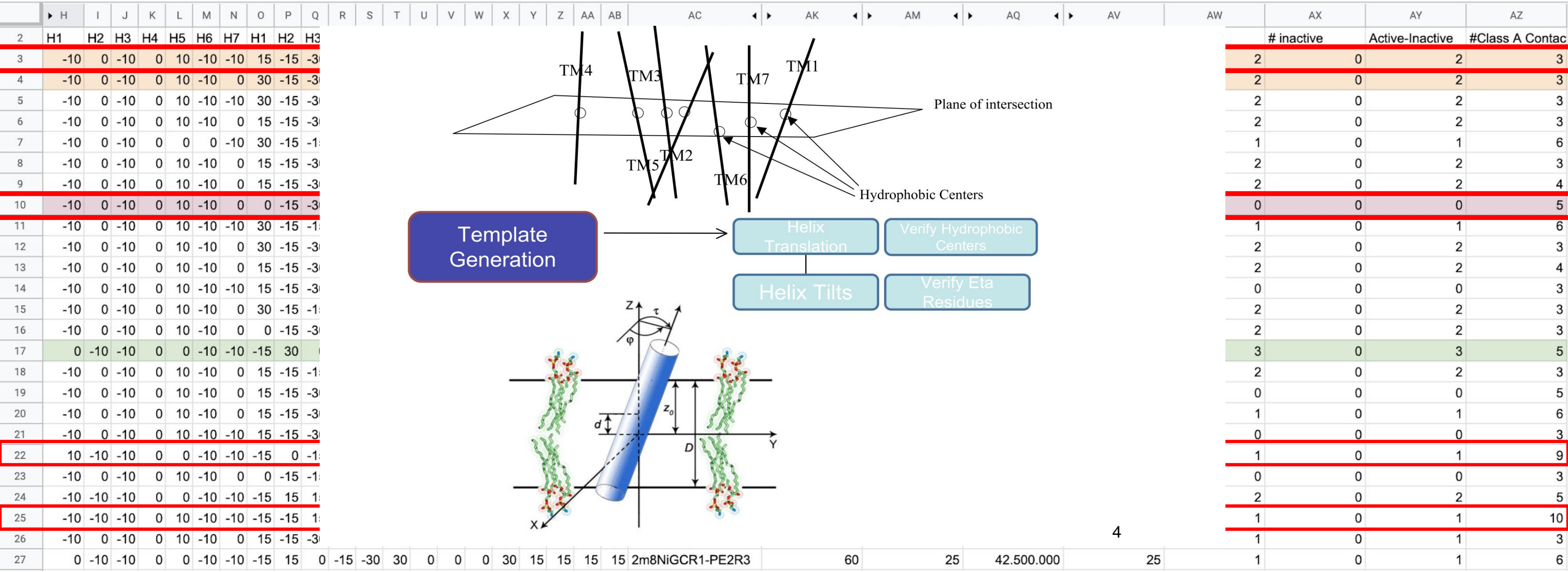
GCR1.mfta



Eta							Source	Individual Energies	
H1	H2	H3	H4	H5	H6	H7	Source	CintraH	CInterH
-90	30	30	60	0	150	-30	PE2R3	492.041.800	-654.036.800
90	0	30	180	0	0	0	PE2R3	467.559.100	-636.980.100
-120	-90	30	180	0	0	0	PE2R3	447.018.200	-632.983.200
-150	90	30	-150	0	150	-30	PE2R3	472.750.100	-627.517.100
120	0	30	90	0	90	-60	PE2R3	392.000.000	-569.016.000

Bray, J. K.; Abrol, R.; Goddard, W. A.; et al. Proceedings of the National Academy of Sciences. 2014

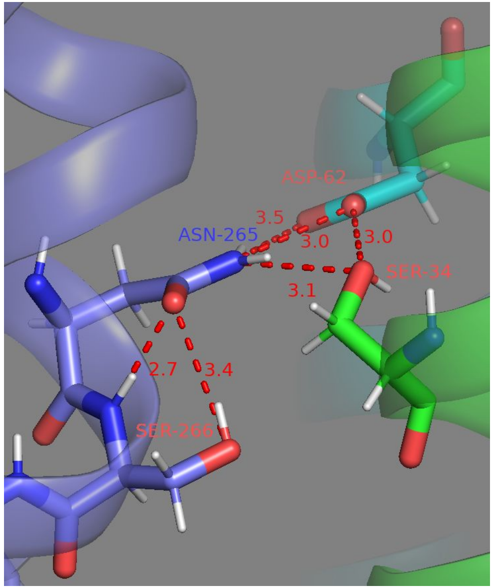
MultiSuperCombiNeutralize
SuperBiHelix

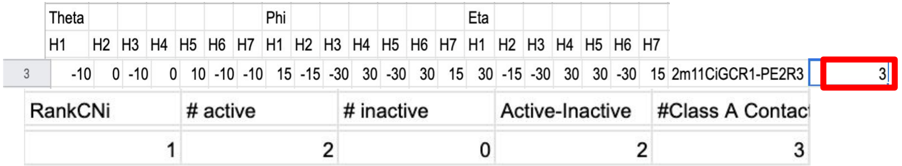


	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AK	AM	AQ	AV	AW	AX	AY	AZ
2	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3																		# inactive	Active-Inactive	#Class A Contac
3	-10	0	-10	0	10	-10	-10	15	-15	-3																	2	0	2	3
4	-10	0	-10	0	10	-10	0	30	-15	-3																	2	0	2	3
5	-10	0	-10	0	10	-10	-10	30	-15	-3																	2	0	2	3
6	-10	0	-10	0	10	-10	0	15	-15	-3																	2	0	2	3
7	-10	0	-10	0	0	0	-10	30	-15	-1																	1	0	1	6
8	-10	0	-10	0	10	-10	0	15	-15	-3																	2	0	2	3
9	-10	0	-10	0	10	-10	0	15	-15	-3																	2	0	2	4
10	-10	0	-10	0	10	-10	0	0	-15	-3																	0	0	0	5
11	-10	0	-10	0	10	-10	-10	30	-15	-1																	1	0	1	6
12	-10	0	-10	0	10	-10	0	30	-15	-3																	2	0	2	3
13	-10	0	-10	0	10	-10	0	15	-15	-3																	2	0	2	4
14	-10	0	-10	0	10	-10	-10	15	-15	-3																	0	0	0	3
15	-10	0	-10	0	10	-10	0	30	-15	-1																	2	0	2	3
16	-10	0	-10	0	10	-10	0	0	-15	-3																	2	0	2	3
17	0	-10	-10	0	0	-10	-10	-15	30																		3	0	3	5
18	-10	0	-10	0	10	-10	0	15	-15	-1																	2	0	2	3
19	-10	0	-10	0	10	-10	0	15	-15	-3																	0	0	0	5
20	-10	0	-10	0	10	-10	0	15	-15	-3																	1	0	1	6
21	-10	0	-10	0	10	-10	-10	15	-15	-3																	0	0	0	3
22	10	-10	-10	0	0	-10	-10	-15	0	-1																	1	0	1	9
23	-10	0	-10	0	10	-10	0	0	-15	-1																	0	0	0	3
24	-10	-10	-10	0	0	-10	-10	-15	15	1																	2	0	2	5
25	-10	-10	-10	0	10	-10	-10	-15	-15	1																	1	0	1	10
26	-10	0	-10	0	10	-10	0	15	-15	-3															4		1	0	1	3
27	0	-10	-10	0	0	-10	-10	-15	15	0	-15	-30	30	0	0	0	30	15	15	15	15	2m8NiGCR1-PE2R3	60	25	42.500.000	25	1	0	1	6

Bray, J. K.; Abrol, R.; Goddard, W. A.; et al. Proceedings of the National Academy of Sciences. 2014

Hydrogen bonding Network: S34(1.50)--N265(7.49)--D62(2.50)



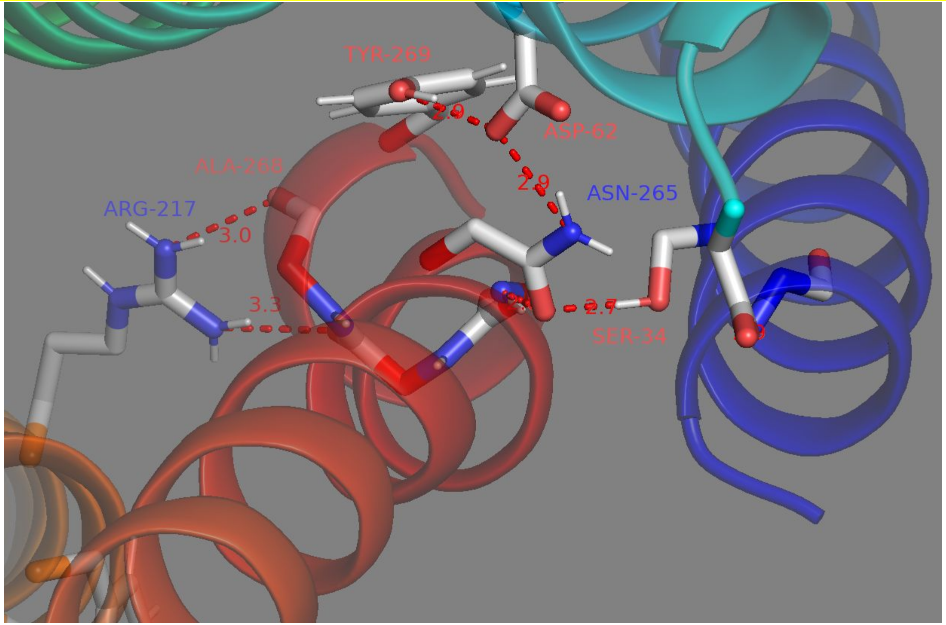


	Theta							Phi							Eta								
	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7		
3	-10	0	-10	0	10	-10	-10	15	-15	-30	30	-30	30	15	30	-15	-30	30	30	-30	15	2m11CiGCR1-PE2R3	3

RankCNi	# active	# inactive	Active-Inactive	#Class A Contac
1	2	0	2	3

	Theta							Phi							Eta								
	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7		
10	-10	0	-10	0	10	-10	0	0	-15	-30	30	-30	30	0	30	0	-30	30	30	-30	30	2m11CiGCR1-PE2R3	6

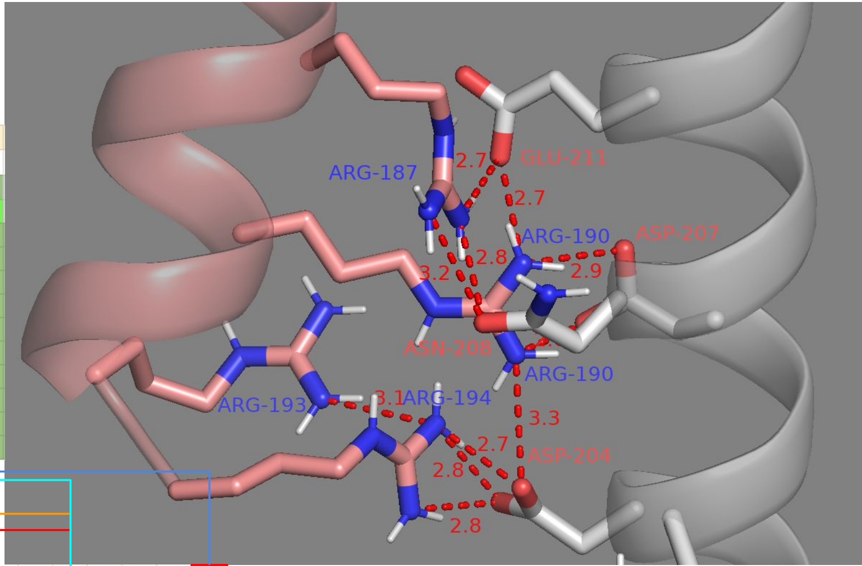
RankCNi	# active	# inactive	Active-Inactive	#Class A Contac
8	0	0	0	5



Conserved H_bonds network among GCR1, and GPCRs de clase A.

D207(6.35)--R190(5.70)--E211(6.39)--R187(5.67)--N208(6.36)
R190(5.70)--D204(6.32)--R194(5.74)--R193(5.73)
Critical for active conformation in human GPCRs.

201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232
	6.30		6.32			6.35	6.36			6.39		6.41									6.50									6.50	
I	T	T	E	T	A	I	Q	L	M	G	I	M	C	V	L	S	V	C	W	S	P	L	L	I	M	M	L	K	M	I	F
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	V	D	Q	F	D	N	R	A	E	L	K	V	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	A	Y	Q	F	D	M	K	A					L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	T	Y	Q	S	D	A	R	A	E	M	K	A	L	N	R	W	G	Y	Y	P	L	I	L	I	G	A	W	A	F	G
D	R	A	Y	Q	F	D	A	R	T	D	M	K	A	L	N	R	W	G	Y	Y	P	L	I	L	I	G	S	W	A	F	G
D	R	A	Y	Q	S	D	A	R	A	E	M	K	A	L	N	R	W	G	Y	Y	P	L	I	L	I	G	A	W	A	F	G



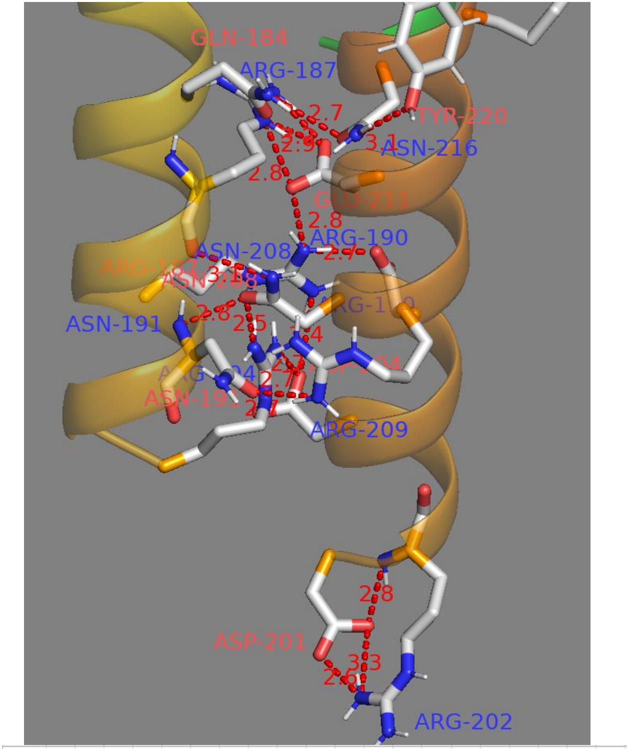
158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194
										5.48		5.50																	5.67			5.70			5.73	5.74
N	L	F	F	A	S	A	F	A	F	L	G	L	L	A	L	T	V	T	F	S	C	N	L	A	T	I	K	A	L	V	S	R	C	R	A	K
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
K	G	K	A	V	H	F	L	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	R	N	A	R	R
T	G	K	A	V	H	F	I	T	F	Y	A	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	N	N	A	T	R
T	G	K	A	I	H	F	I	T	F	Y	M	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	S	M	L	K	N	A	R	R
T	G	K	A	V	H	F	I	T	F	Y	V	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	R	M	L	N	N	A	T	R
T	G	K	A	I	H	F	I	T	F	Y	M	P	L	W	G	A	I	L	Y	N	G	F	T	Y	F	Q	V	I	S	M	L	K	N	A	R	R

If 6 - 3 interactions are broken and there are 5 - 6 interactions, can it be an indication of inactive state of GCR1?

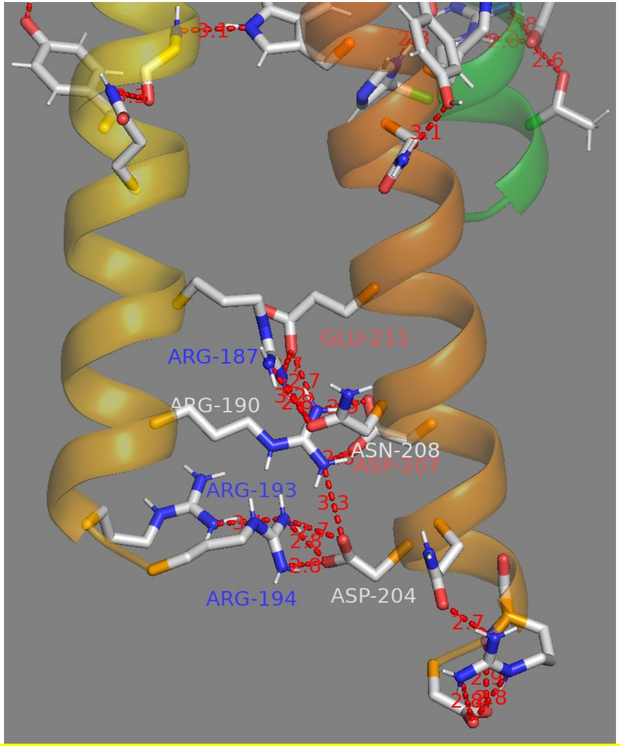
D204(6.32)--R194(5.74)--R190(5.70)--E211(6.39)--R187(5.67)--N208(6.36)--N191(5.71)--R209(6.37)

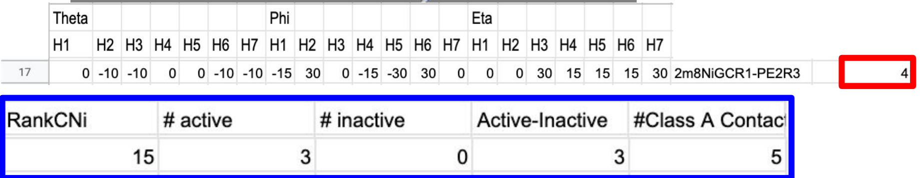
R193(5.73)--R194(5.74)--D204---R190(5.70)--E211(6.39)--R187(5.67)--N208(6.36)

Salt bridges interactions critical for active conformation in human GPCRs.



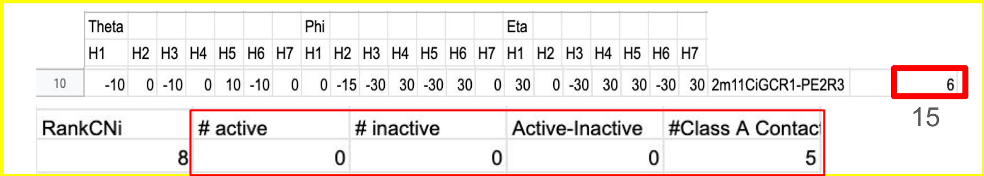
E211(6.39 or 6.30)





	Theta							Phi							Eta								
	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7		
17	0	-10	-10	0	0	-10	-10	-15	30	0	-15	-30	30	0	0	0	30	15	15	15	30	2m8NiGCR1-PE2R3	4

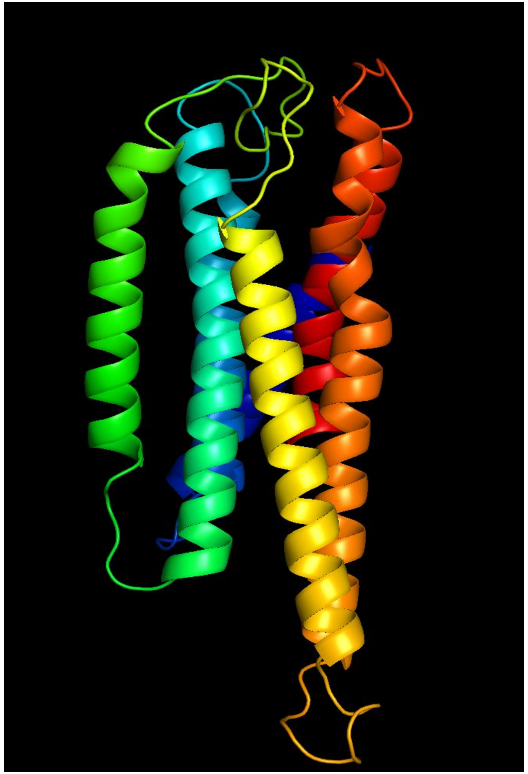
RankCNi	# active	# inactive	Active-Inactive	#Class A Contact
15	3	0	3	5

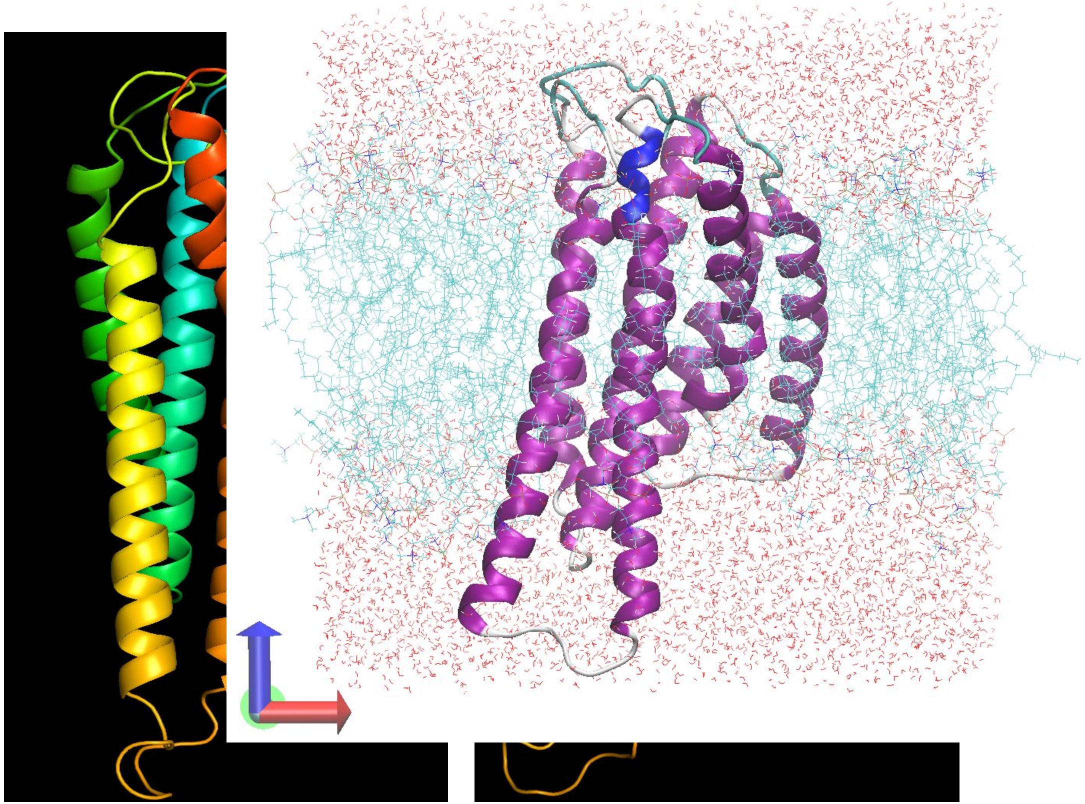


	Theta							Phi							Eta								
	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7	H1	H2	H3	H4	H5	H6	H7		
10	-10	0	-10	0	10	-10	0	0	-15	-30	30	-30	30	0	30	0	-30	30	30	-30	30	2m11CiGCR1-PE2R3	6

RankCNi	# active	# inactive	Active-Inactive	#Class A Contact
8	0	0	0	5

04Ni_GPCR





06Ci.bgf to 06Ci_GCR1

↓

1 Loops translation

1.1 06Ci.bgf alignment to GCR1

↓

1 Loops translation

1.2 Loops + TMs connections

↓

2 pdb to bgf

Annealing procedure preparation

↓

2 pdb to bgf

Questions about Annealing-procedure preparation

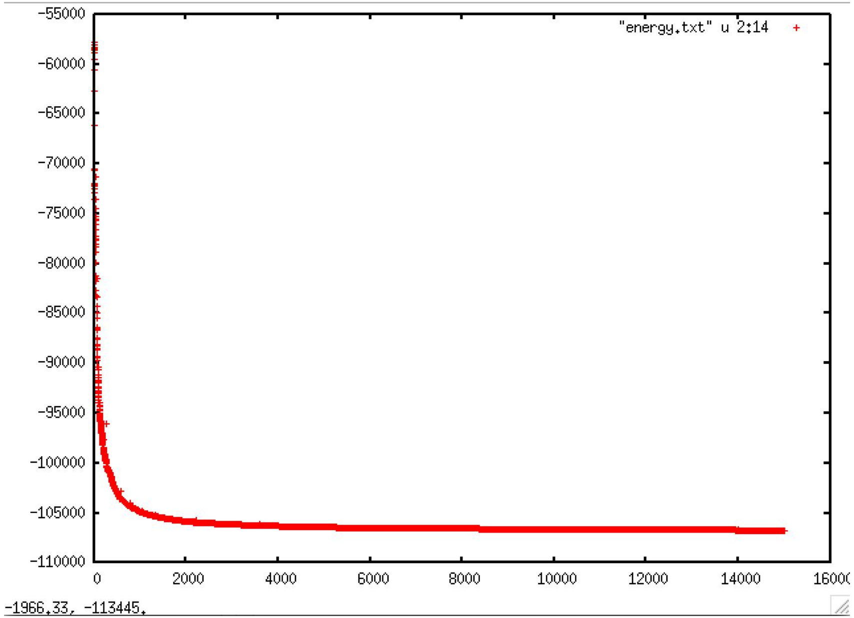
↓

3 Simulated annealing

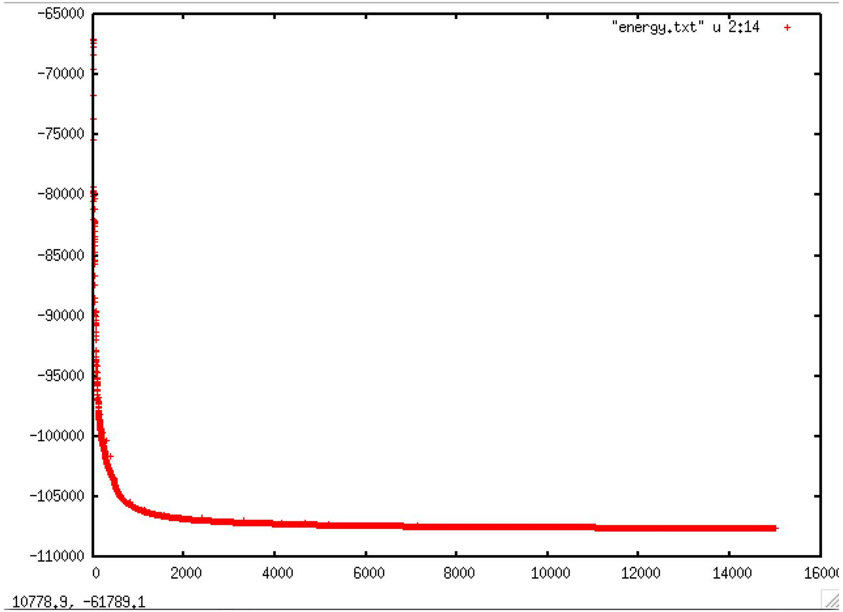
Results

04_GCR1 Vs 06_GCR1 min02.log files

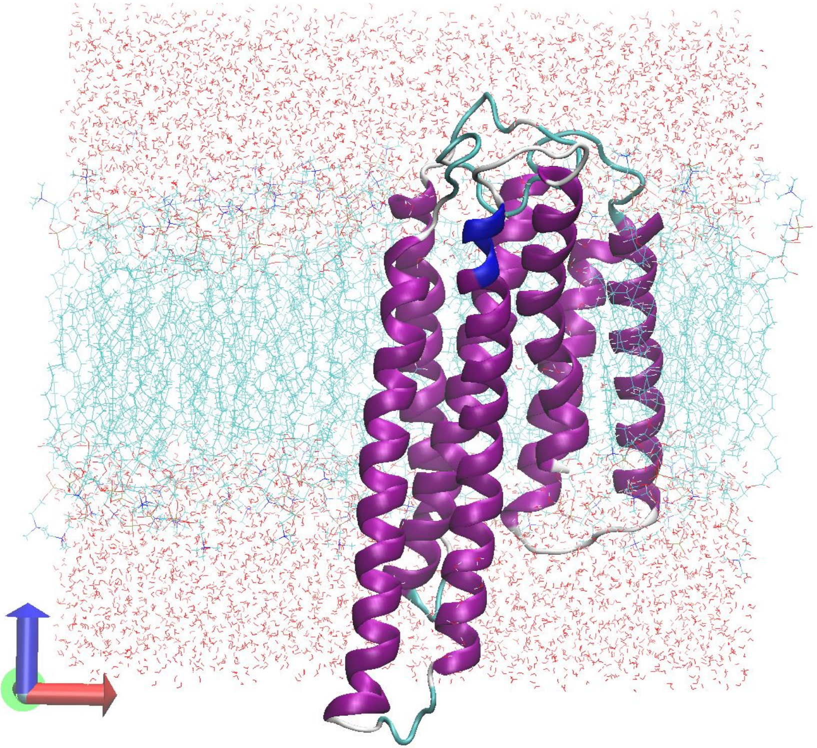
04Ni_GCR1



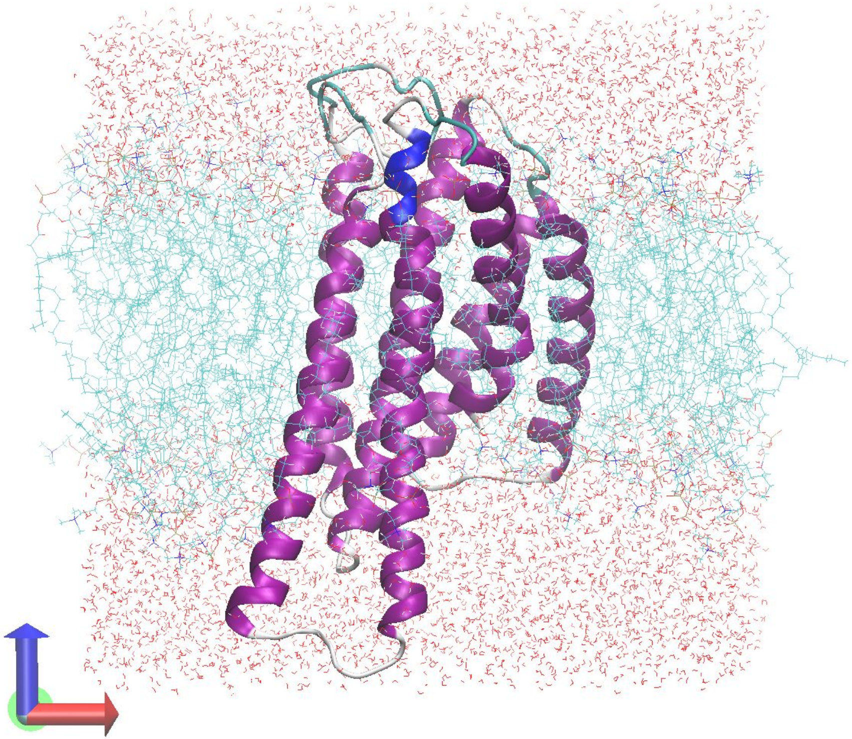
06Ci_GCR1



04_GCR1 Vs 06_GCR1 min02.dcd files



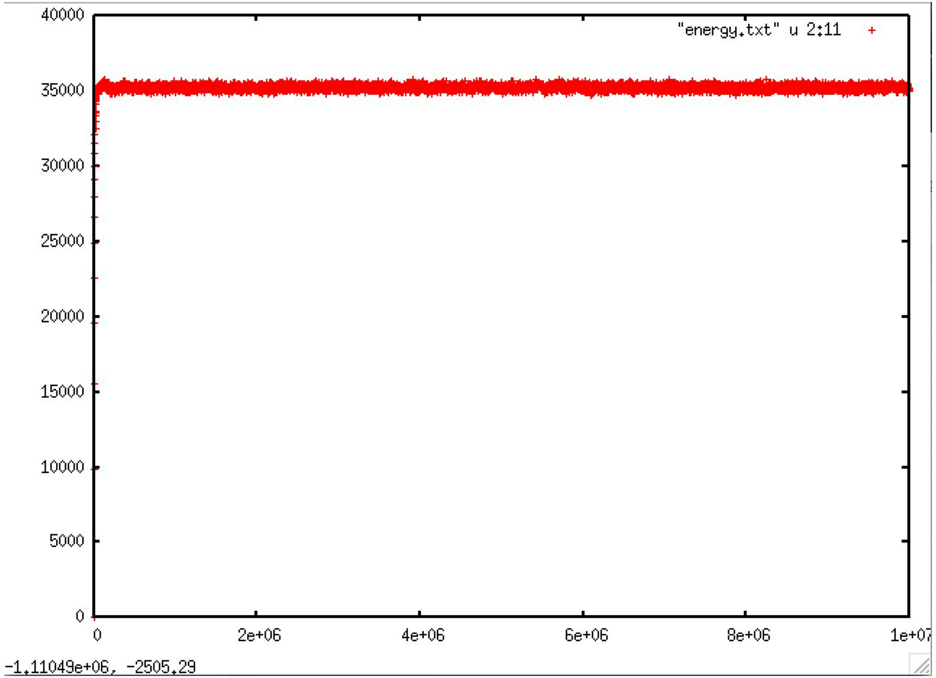
04Ni_GCR1



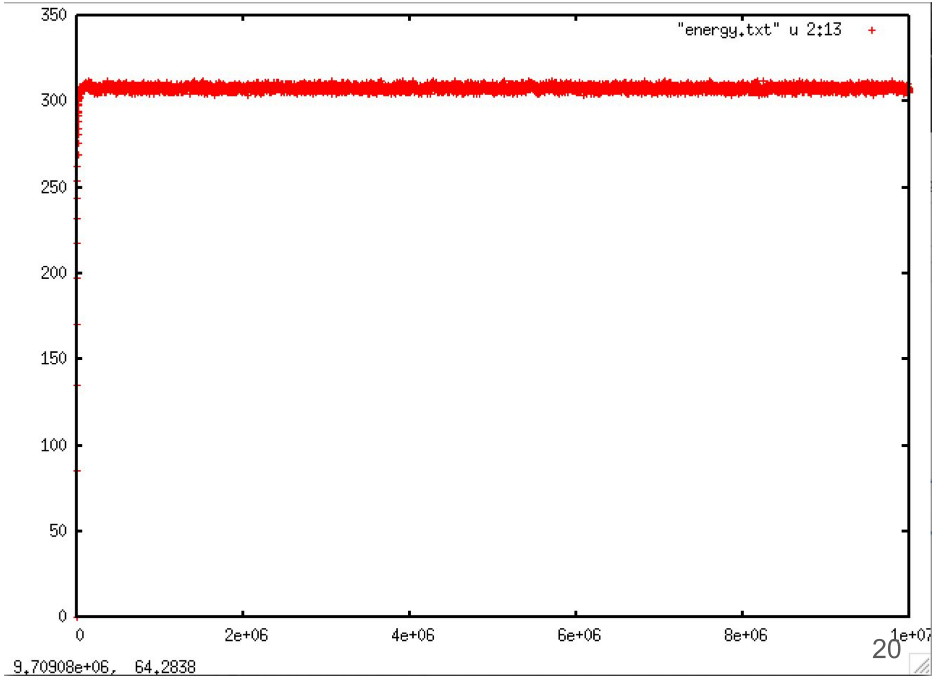
06Ci_GCR1

04_GCR1 eq02.log analysis

TS : kinetic

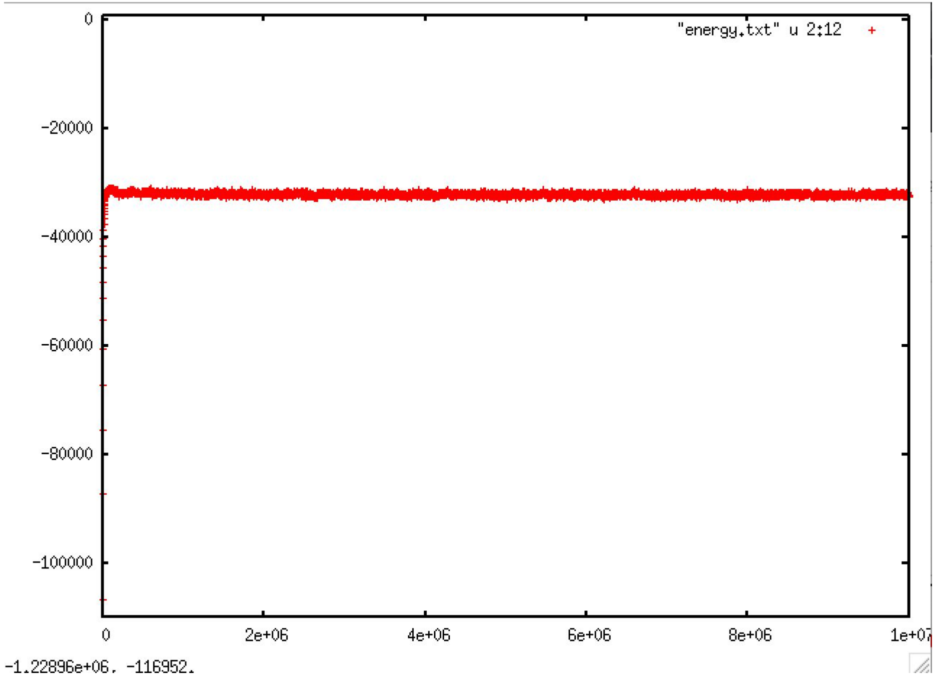


TS : temp



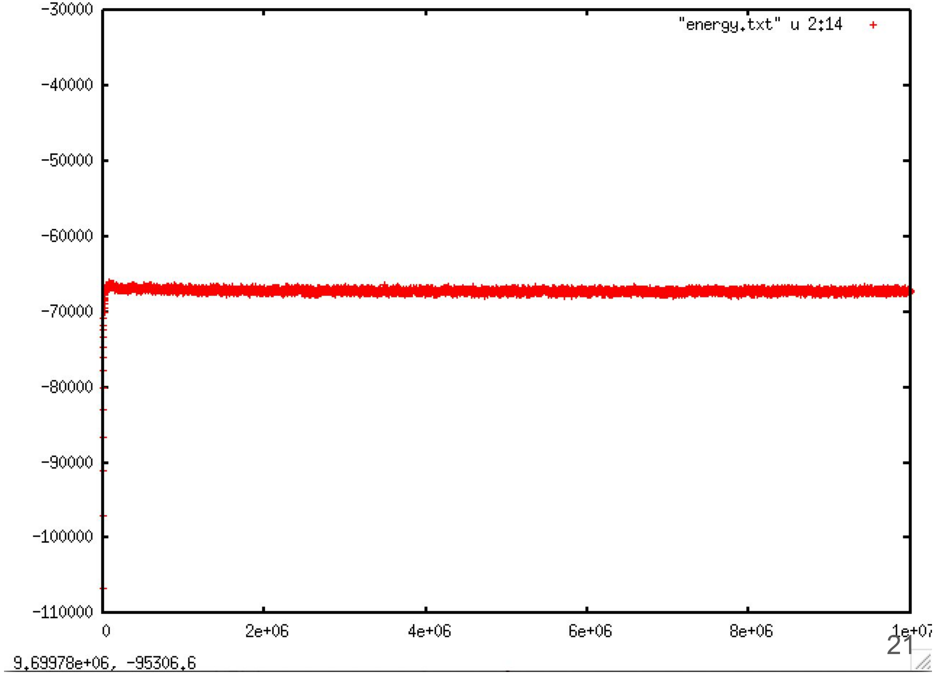
04_GCR1 eq02.log analysis

TS : total



-1.22896e+06, -116952.

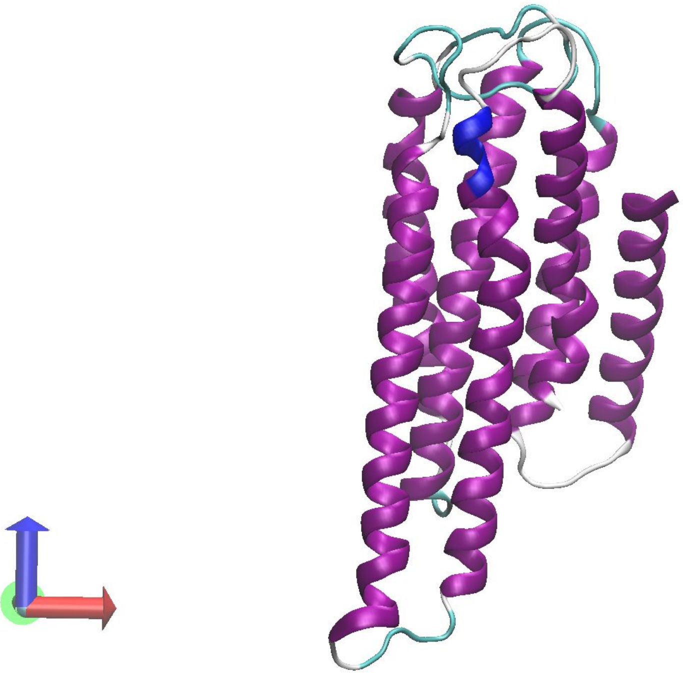
TS : potential



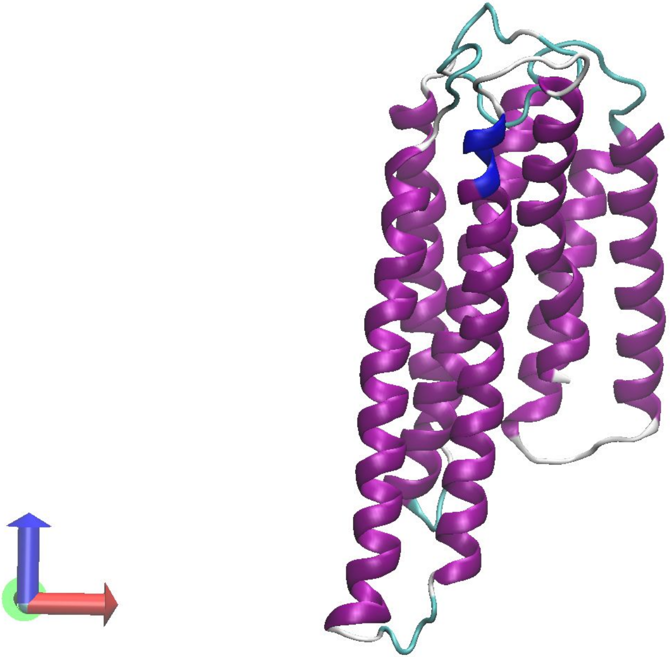
9.69978e+06, -95306.6

04Ni_GCR1 min02.dcd

Starting point

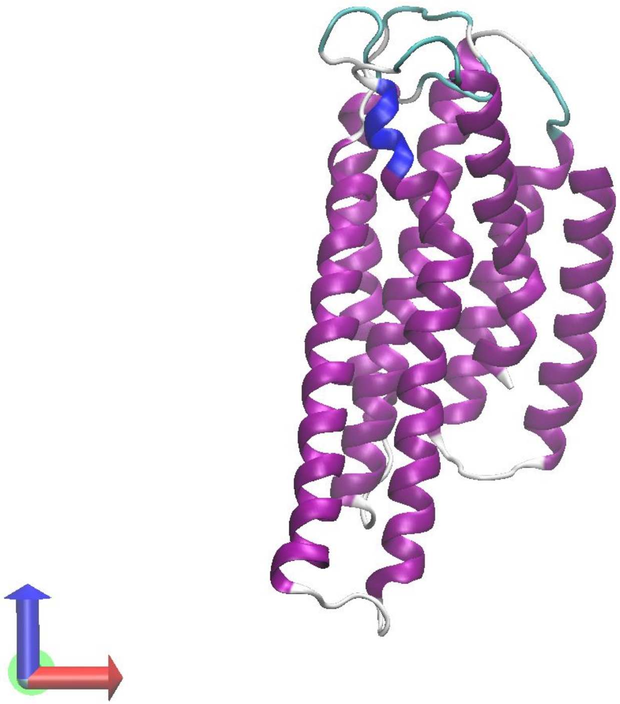


Final point

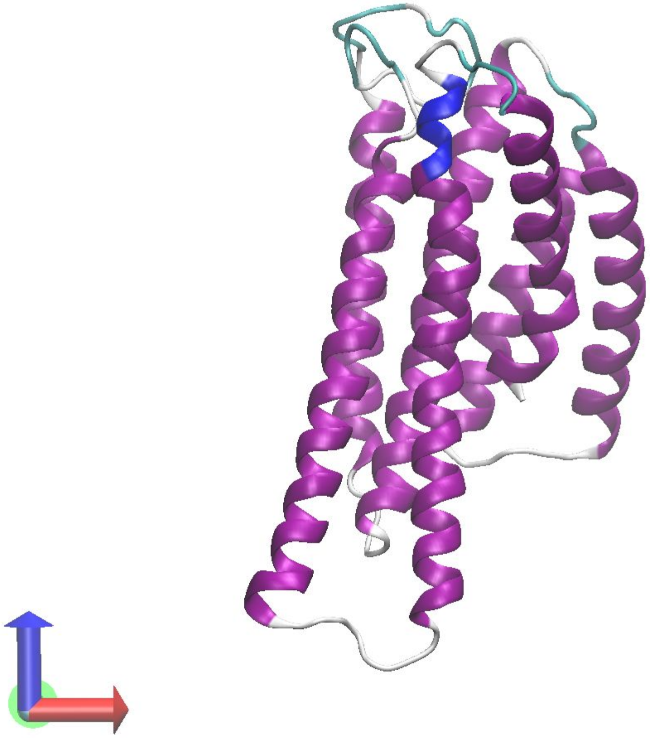


06Ci_GCR1 min02.dcd

Starting point

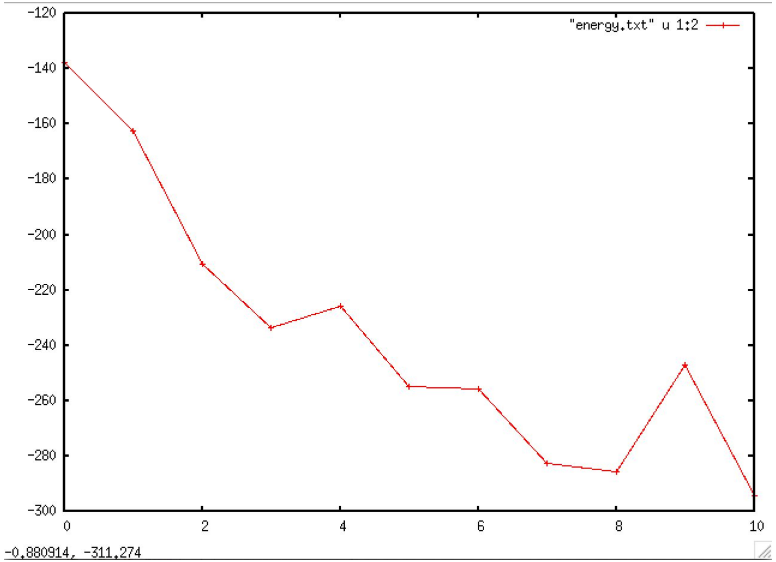


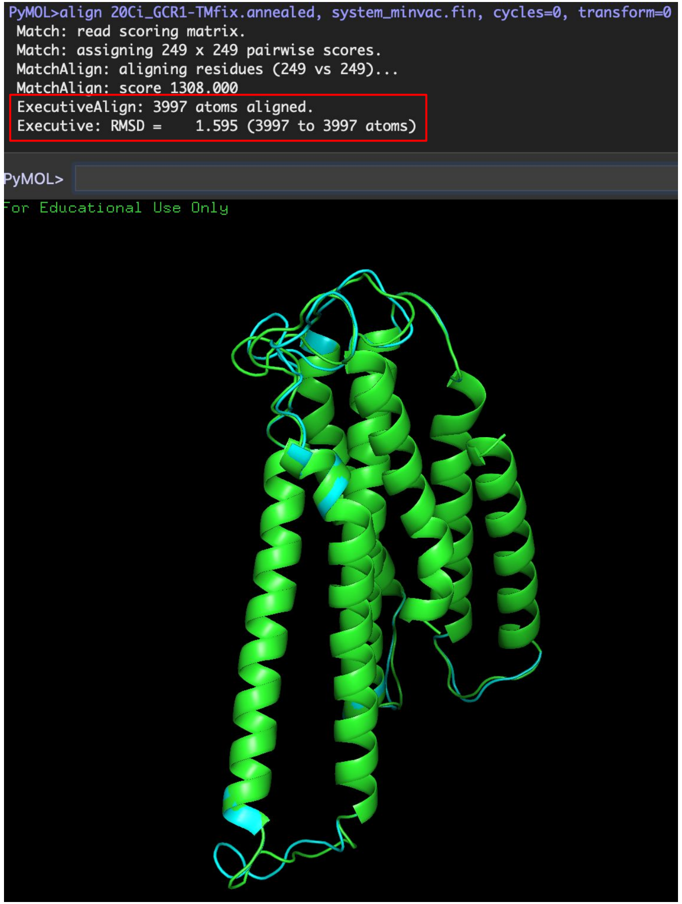
Final point



alignment and RMSD between between 20Ci-GCR1_noH_TMfix.annealed and system_minvac.fin

0	-137.885
1	-162.693
2	-210.722
3	-233.652
4	-225.566
5	-254.661
6	-255.747
7	-282.483
8	-285.503
9	-246.771
10	-294.057

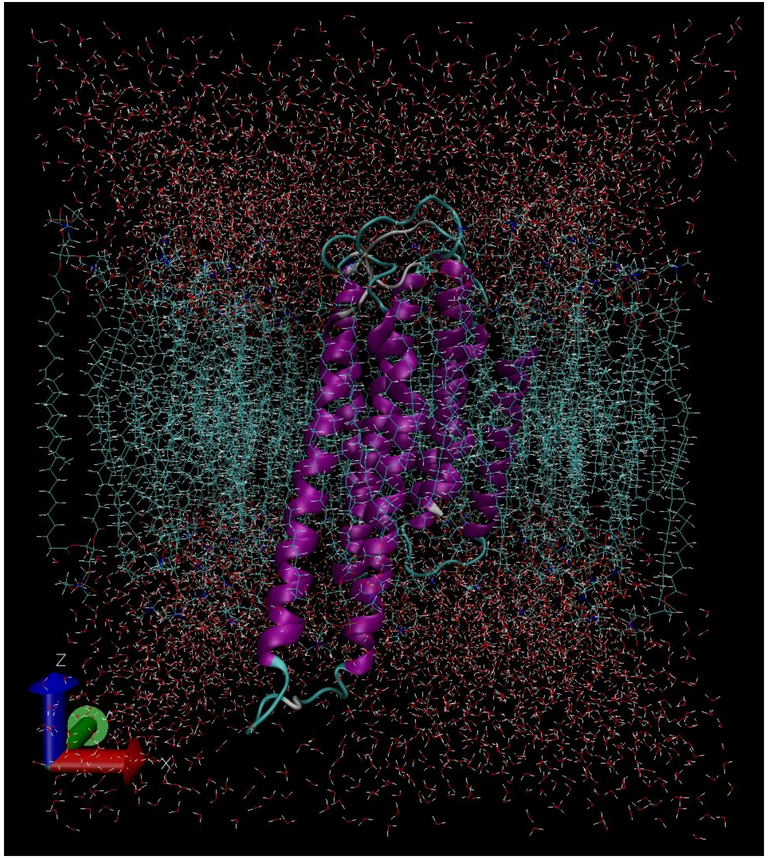




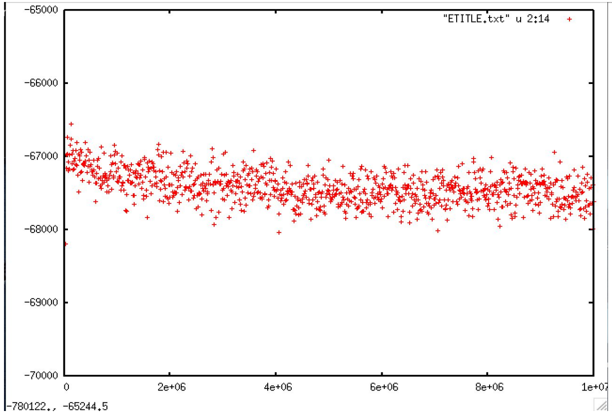
```
PyMOL>align 20Ci_GCR1-TMfix.annealed, system_minvac.fin, cycles=0, transform=0
 Match: read scoring matrix.
 Match: assigning 249 x 249 pairwise scores.
 MatchAlign: aligning residues (249 vs 249)...
 MatchAlign: score 1308.000
 ExecutiveAlign: 3997 atoms aligned.
 Executive: RMSD =    1.595 (3997 to 3997 atoms)
```

20Ci_gcr1 Starting structure (from minimized simulated annealing structure)

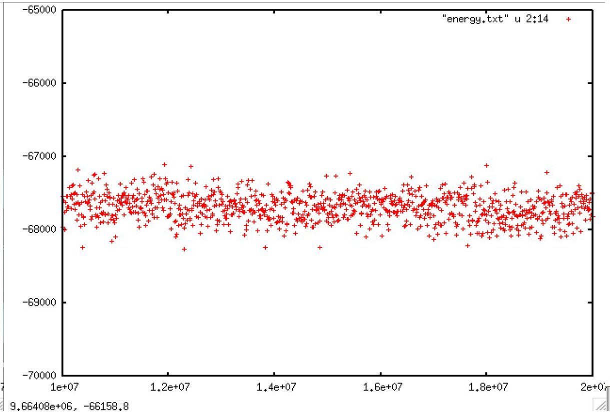
yourprot-lig+POPC+wat+NaCl.pdb



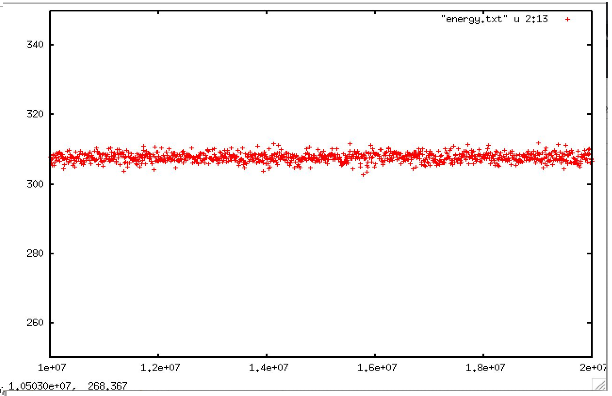
Equilibrate 2 Potential Energy



Equilibrate 3 Potential Energy



Equilibrate 3 Temperature

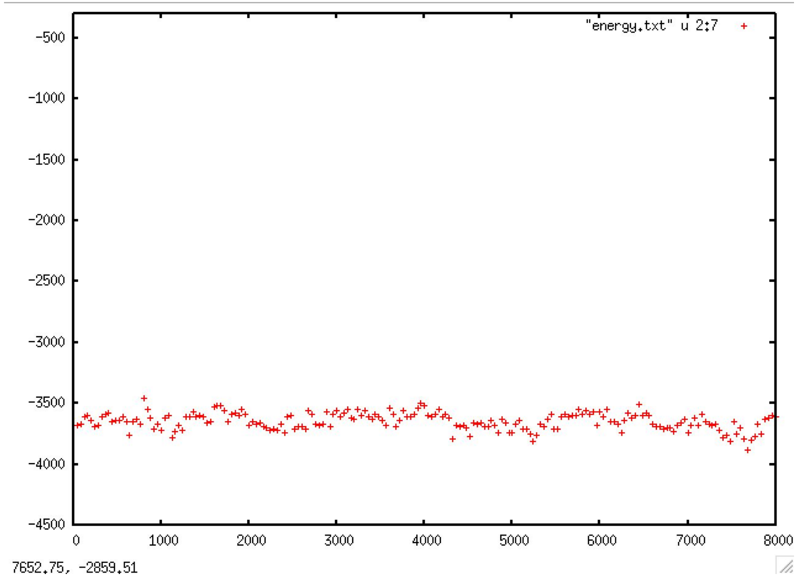


Protein_Energy 20Ci_GCR1

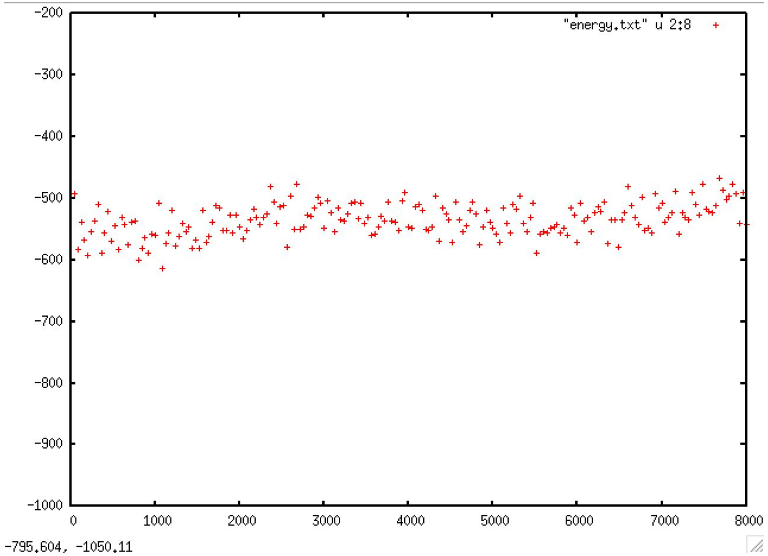
ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW	BOUNDARY	MISC	KINETIC	TOTAL
1	2	3	4	5	6	7	8	9	10	11	12

TEMP	TOTAL2	TOTAL3	TEMPAVG
13	14	15	16

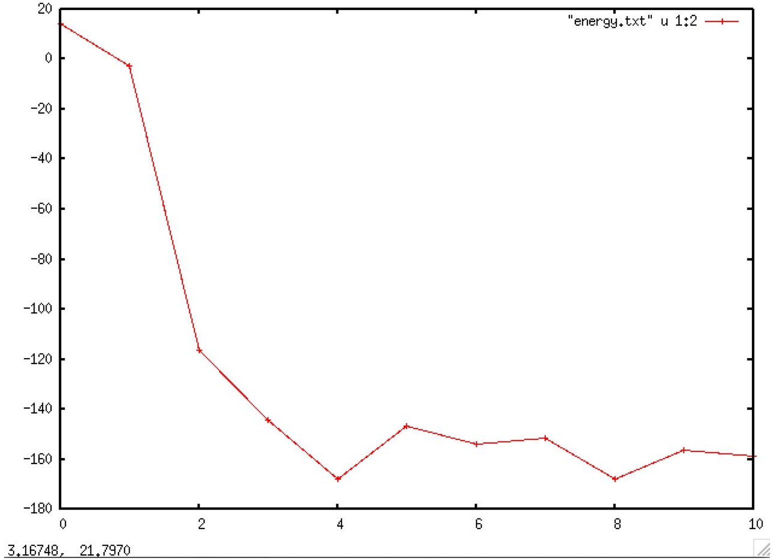
ELECT



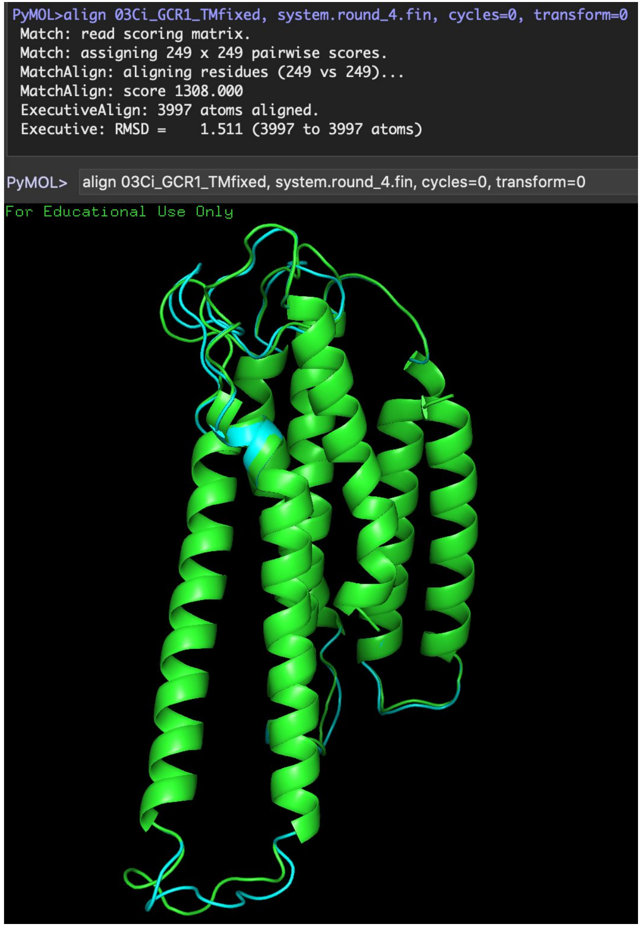
VDW



alignment between system.round_4.fin.bgf and 03Ci-GCR1_TMfixed.bgf



0	14.02
1	-2.64055
2	-116.409
3	-144.018
4	-167.795
5	-146.396
6	-153.773
7	-151.435
8	-167.714
9	-156.242
10	-158.664



```
PyMOL>align 03Ci_GCR1_TMfixed, system.round_4.fin, cycles=0, transform=0
 Match: read scoring matrix.
 Match: assigning 249 x 249 pairwise scores.
 MatchAlign: aligning residues (249 vs 249)...
 MatchAlign: score 1308.000
 ExecutiveAlign: 3997 atoms aligned.
 Executive: RMSD =    1.511 (3997 to 3997 atoms)
```

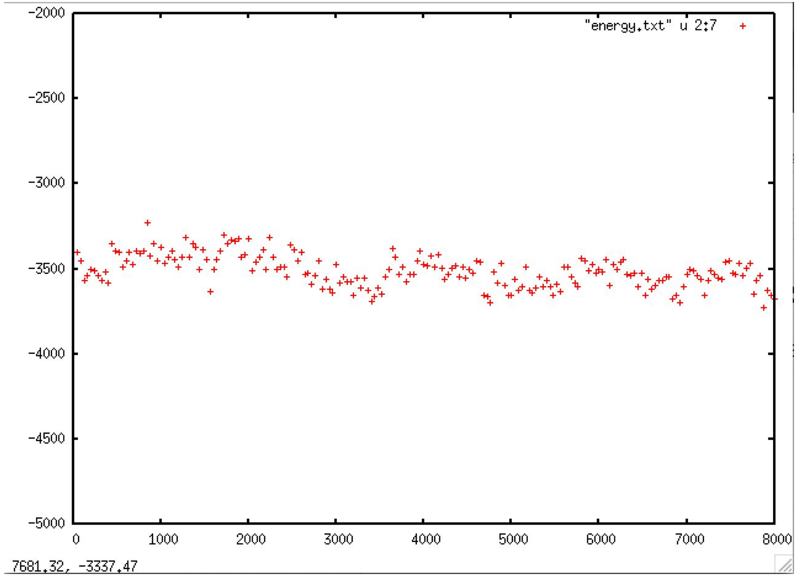
```
PyMOL> align 03Ci_GCR1_TMfixed, system.round_4.fin, cycles=0, transform=0
```

Protein_Energy 03Ci_GCR1-

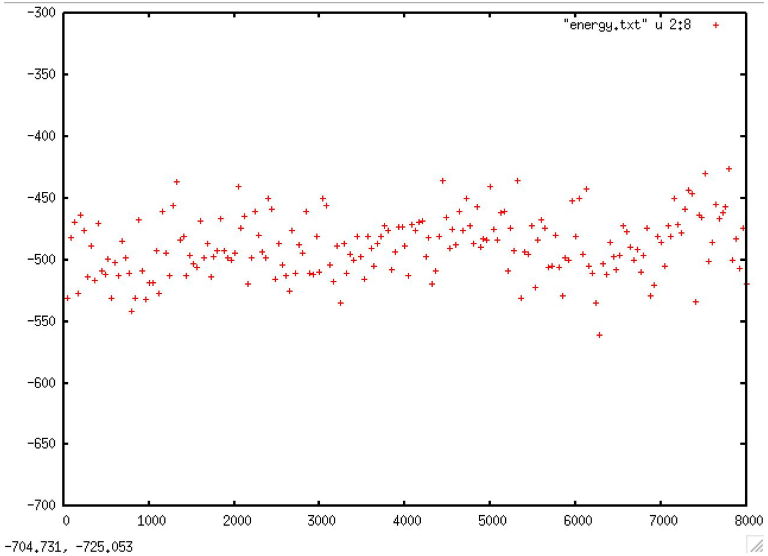
ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW	BOUNDARY	MISC	KINETIC	TOTAL
1	2	3	4	5	6	7	8	9	10	11	12

TEMP	TOTAL2	TOTAL3	TEMPAVG
13	14	15	16

ELECT



VDW



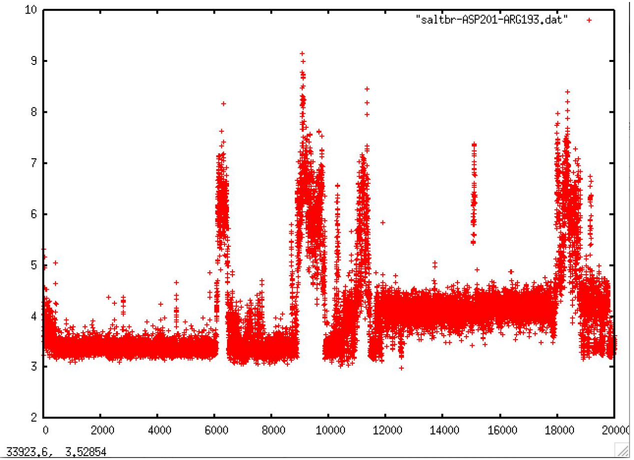
03Ci_GCR1

10 stable salt bridges.
2 Marginal salt bridges.
4 No salt bridges.

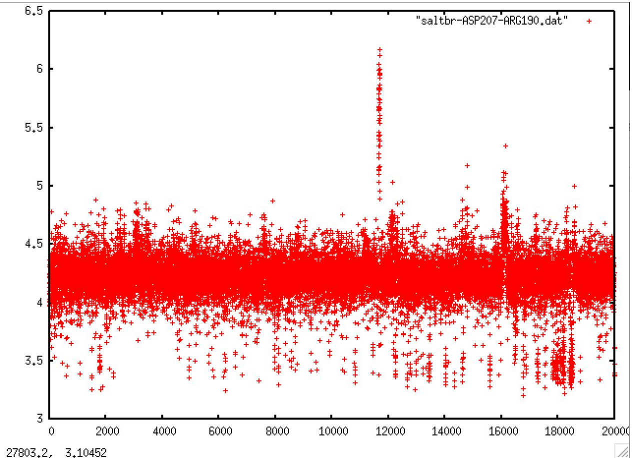
Total 16

03Ci_GCR1

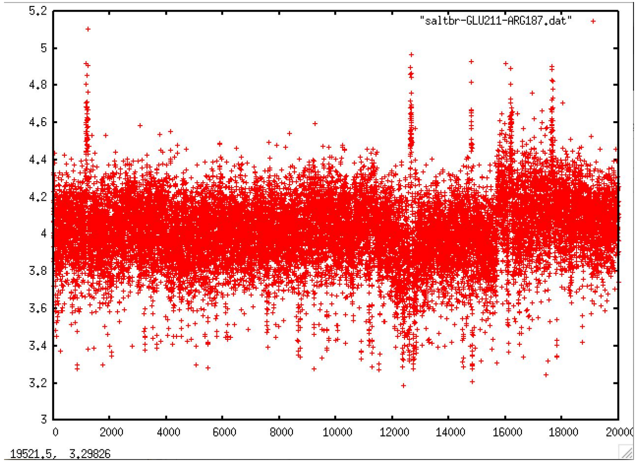
saltbr-ASP201-ARG193.dat (IC3-5.73)



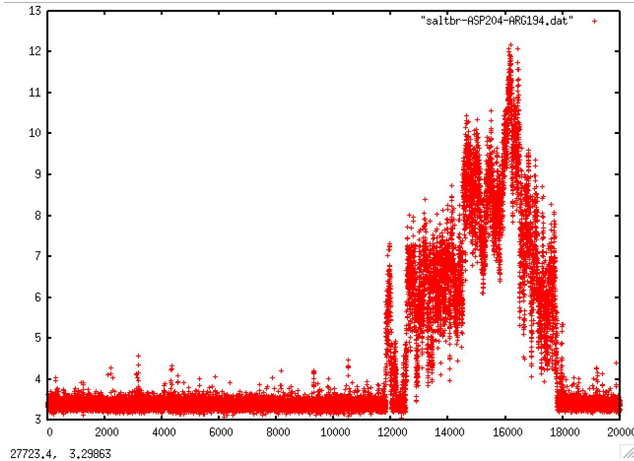
saltbr-ASP207-ARG190.dat (6.26-5.70)



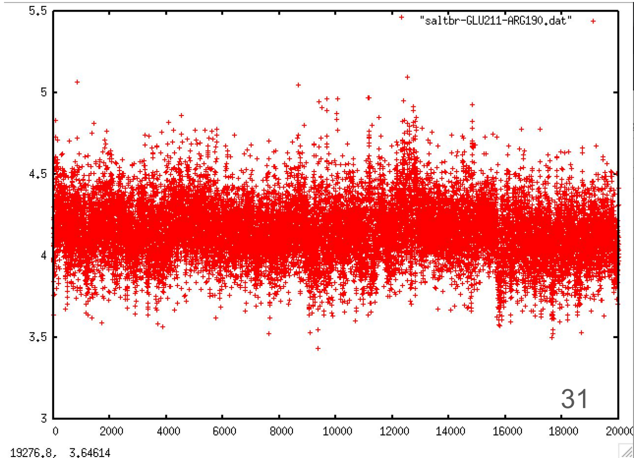
saltbr-GLU211-ARG187.dat (6.30 - 5.67)



saltbr-ASP204-ARG194.dat (6.23-5.74)

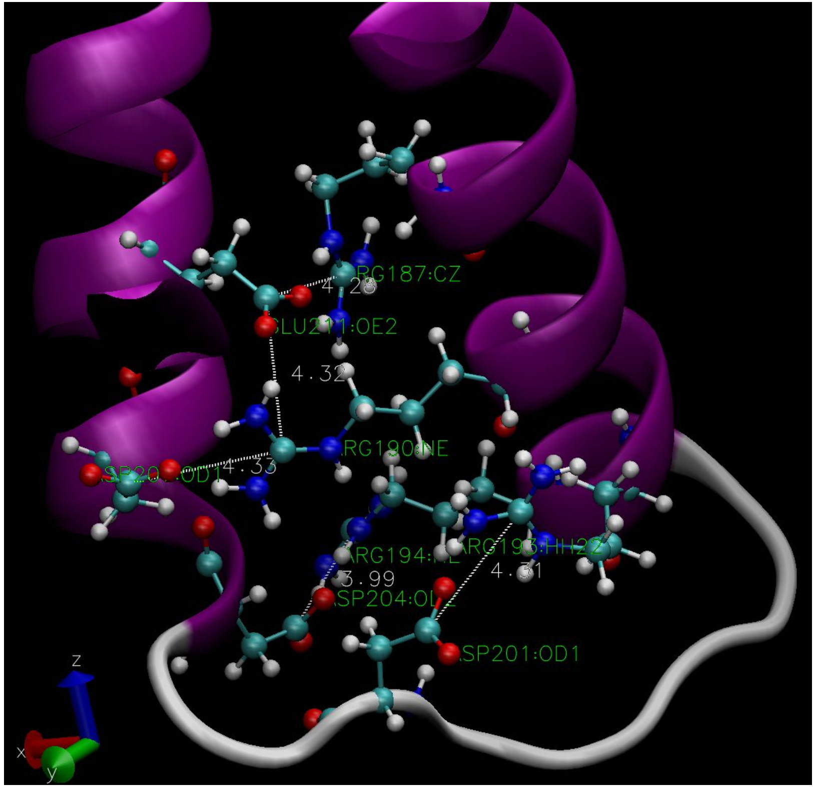


saltbr-GLU211-ARG190.dat (6.30 - 5.70)

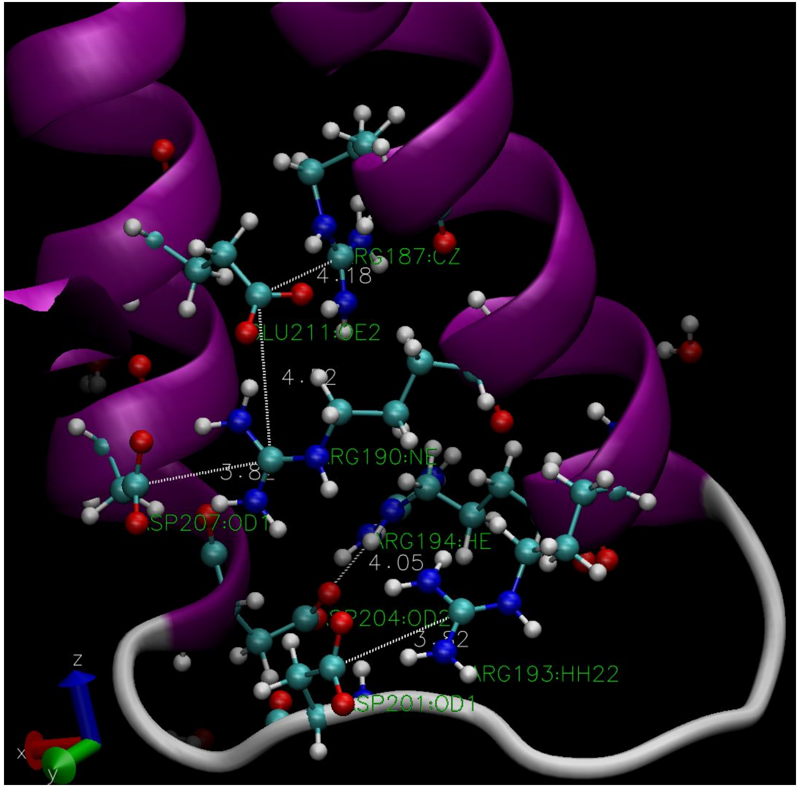


Protein_Energy 03Ci_GCR1-20ns-helix_restrained (for a total of 60ns_helix-restrained)

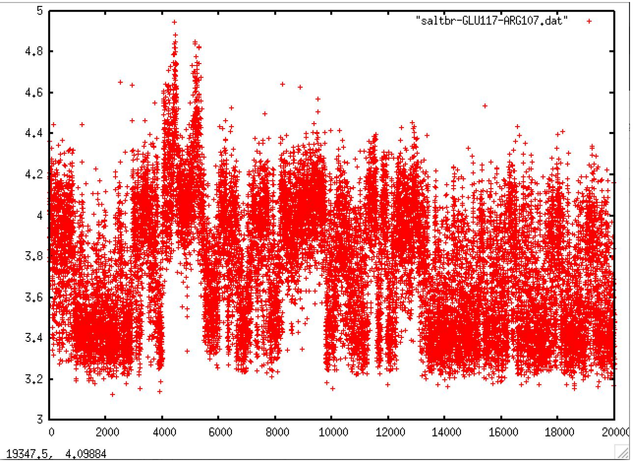
Starting point



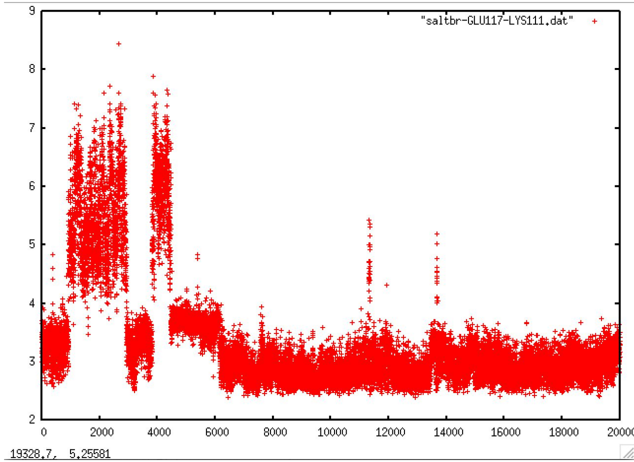
Final point



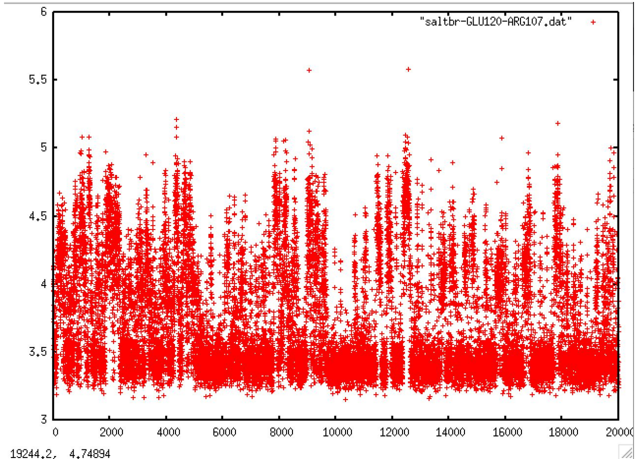
saltbr-GLU117-ARG107.dat (4.39-3.52)



saltbr-GLU117-LYS111.dat (4.39-IC2)

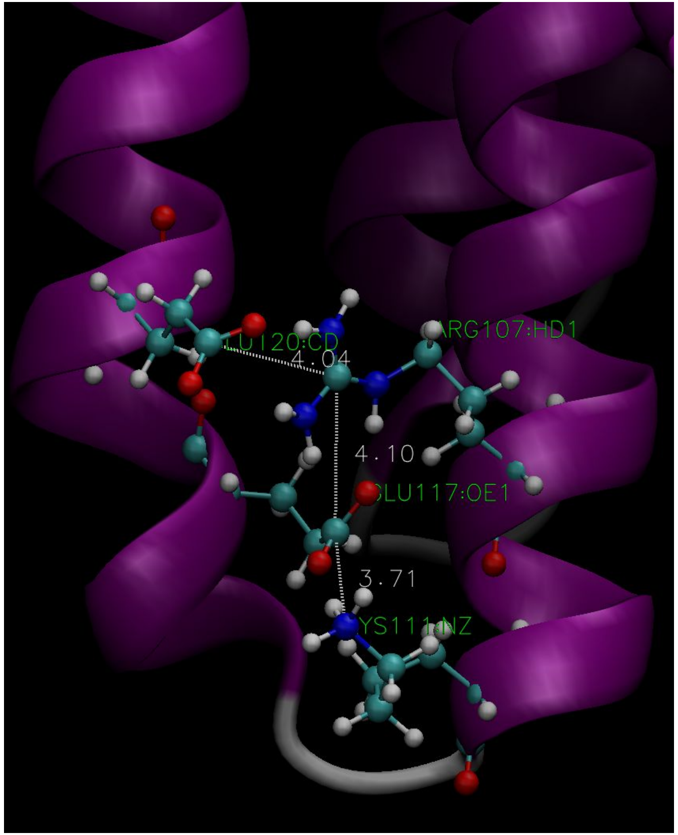


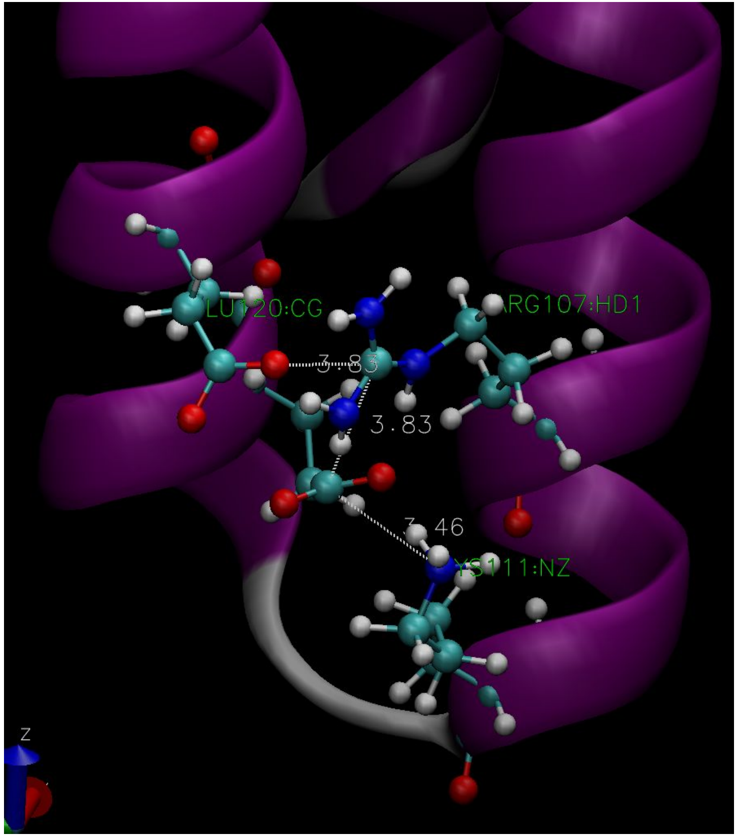
saltbr-GLU120-ARG107.dat (4.42 - 3.52)

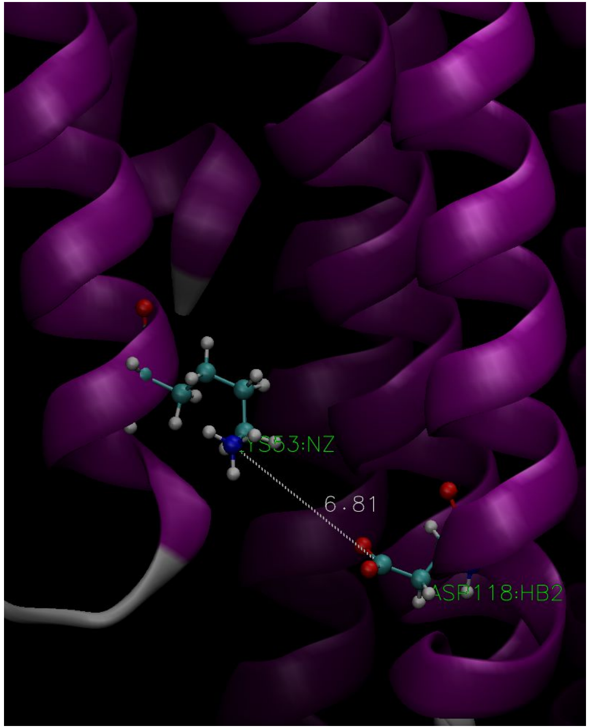


Protein_Energy 3Ci_GCR1-20ns-helix_restrained (for a total of 60ns_helix-restrained)

(4.39-3.52) (4.39-IC2) (4.42 - 3.52)

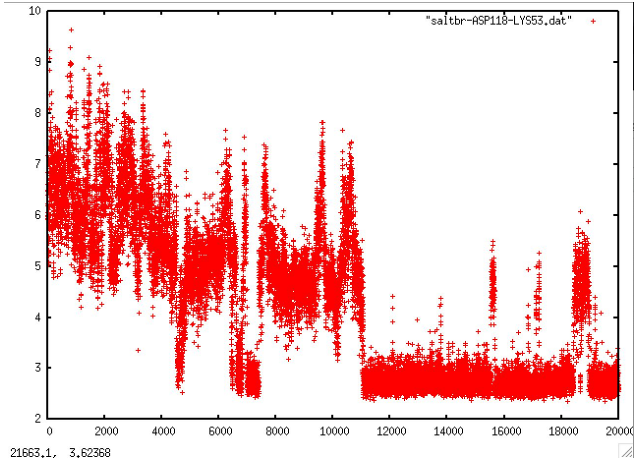




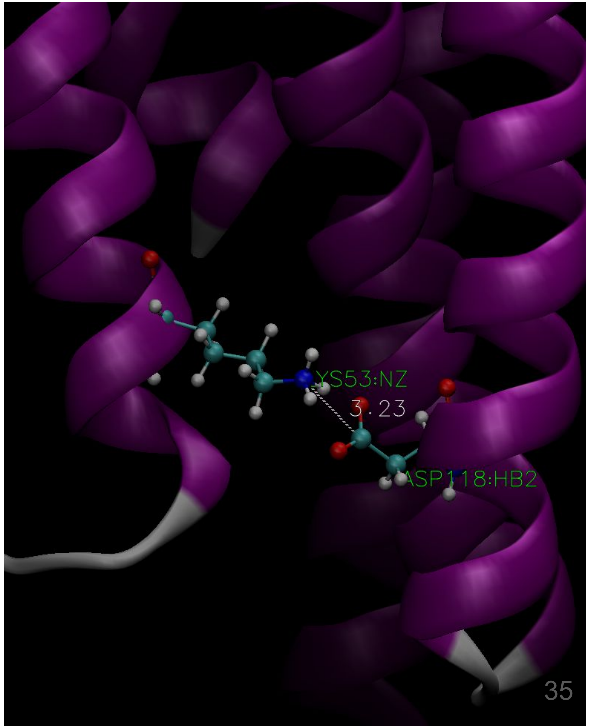


Starting point

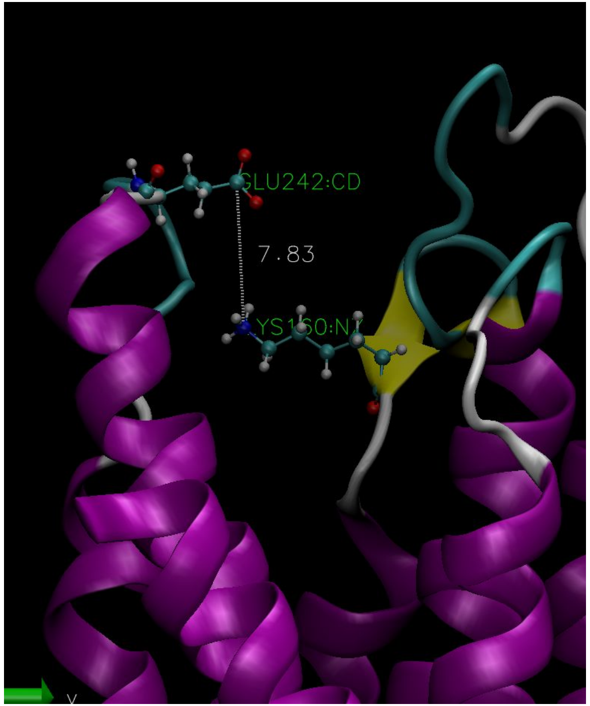
saltbr-ASP118-LYS53.dat (4.40-2.41)



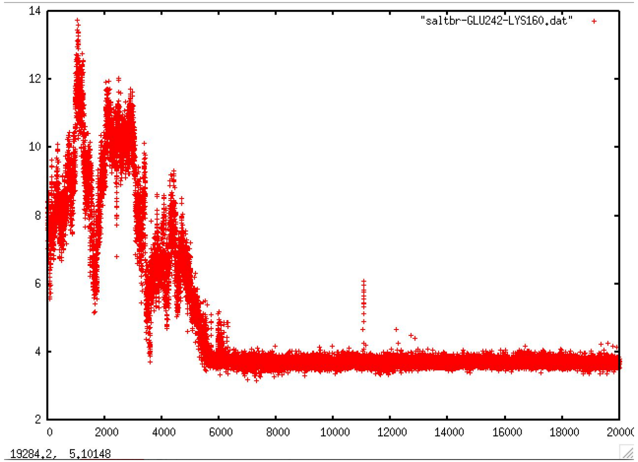
Final point

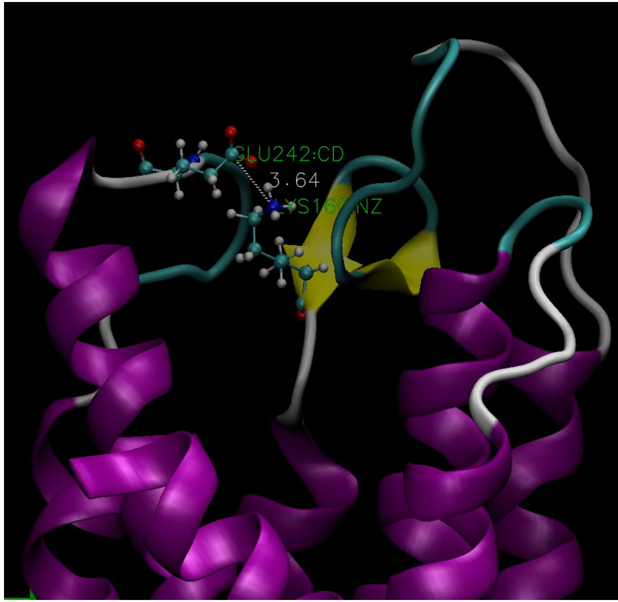


Starting point



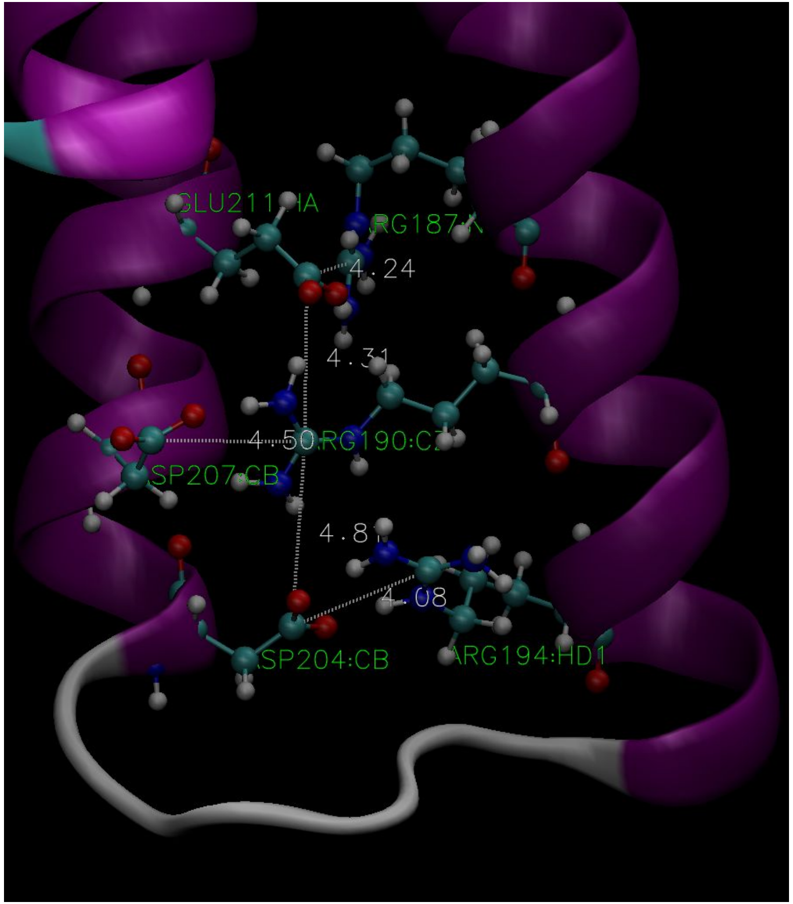
saltbr-GLU242-LYS160.dat (EC3-EC2)



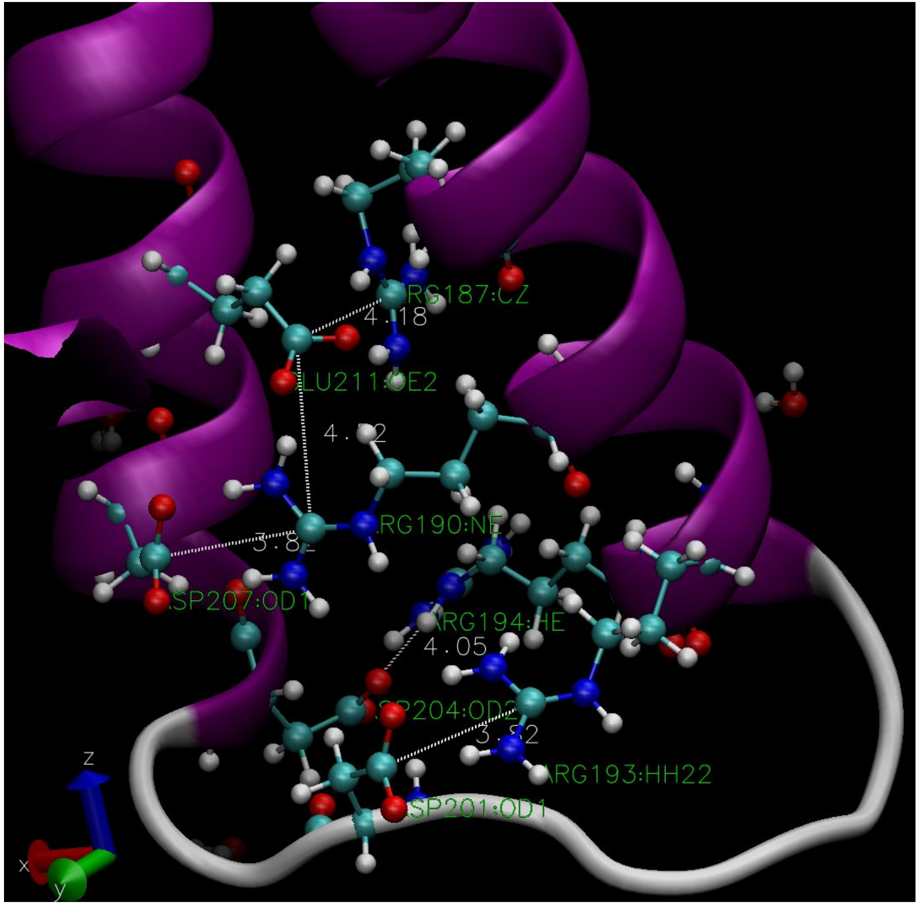


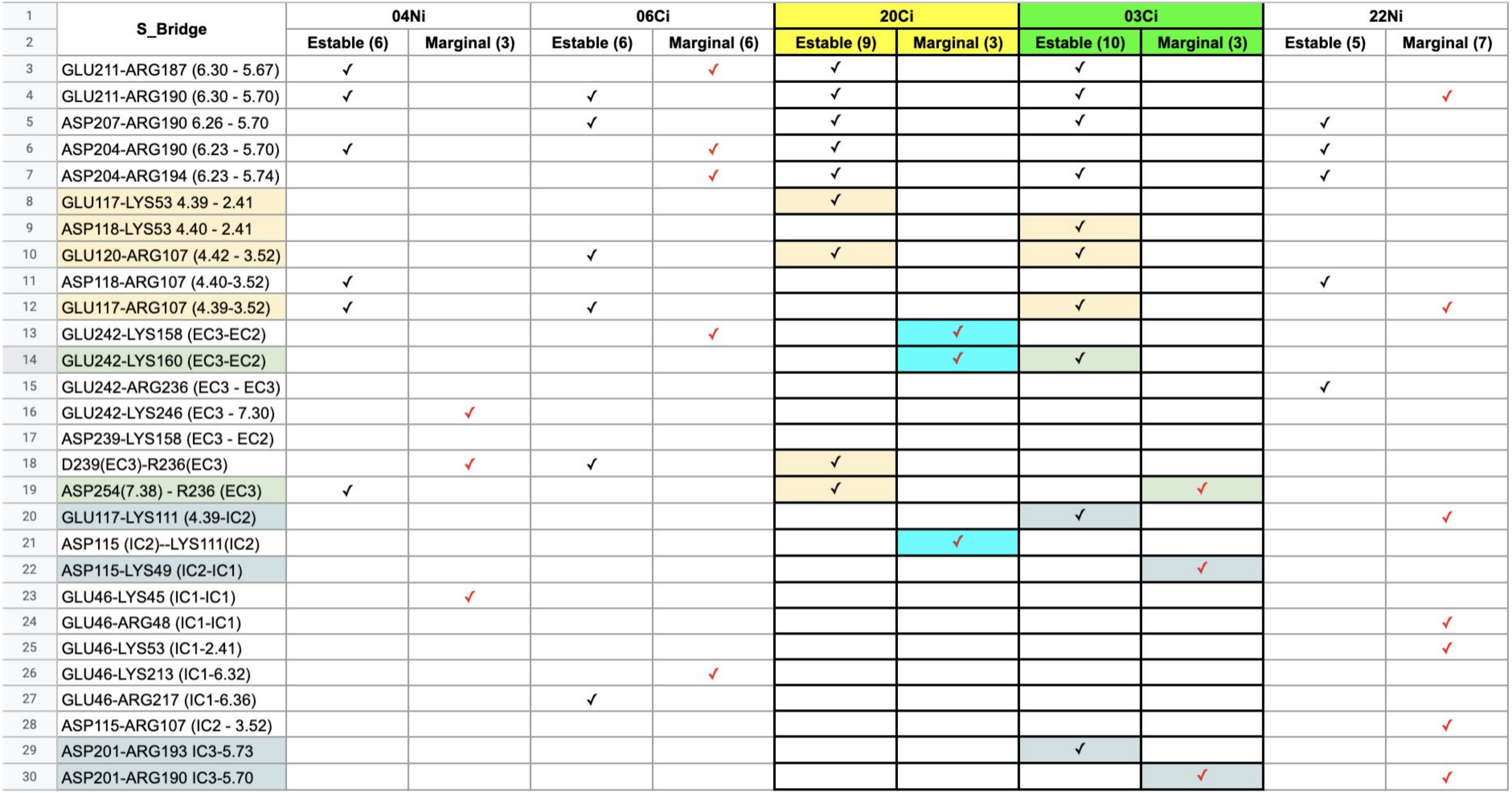
Final point

20Ci


GLU211:HA
RG187:N
4.24
4.31
4.50
RG190:CZ
SP207:CB
4.81
4.08
SP204:CB
ARG194:HD1

03Ci


RG187:CZ
4.18
LU211:OE2
4.72
RG190:NE
3.82
SP207:OD1
RG194:HE
4.05
SP204:OD2
3.82
RG193:HH22
SP201:OD1
z
x
y



1	S_Bridge	04Ni		06Ci		20Ci		03Ci		22Ni	
2		Estable (6)	Marginal (3)	Estable (6)	Marginal (6)	Estable (9)	Marginal (3)	Estable (10)	Marginal (3)	Estable (5)	Marginal (7)
3	GLU211-ARG187 (6.30 - 5.67)	✓			✓	✓		✓			
4	GLU211-ARG190 (6.30 - 5.70)	✓		✓		✓		✓			✓
5	ASP207-ARG190 6.26 - 5.70			✓		✓		✓		✓	
6	ASP204-ARG190 (6.23 - 5.70)	✓			✓	✓				✓	
7	ASP204-ARG194 (6.23 - 5.74)				✓	✓		✓		✓	
8	GLU117-LYS53 4.39 - 2.41					✓					
9	ASP118-LYS53 4.40 - 2.41							✓			
10	GLU120-ARG107 (4.42 - 3.52)			✓		✓		✓			
11	ASP118-ARG107 (4.40-3.52)	✓								✓	
12	GLU117-ARG107 (4.39-3.52)	✓		✓				✓			✓
13	GLU242-LYS158 (EC3-EC2)				✓		✓				
14	GLU242-LYS160 (EC3-EC2)						✓	✓			
15	GLU242-ARG236 (EC3 - EC3)									✓	
16	GLU242-LYS246 (EC3 - 7.30)		✓								
17	ASP239-LYS158 (EC3 - EC2)										
18	D239(EC3)-R236(EC3)		✓	✓		✓					
19	ASP254(7.38) - R236 (EC3)	✓				✓			✓		
20	GLU117-LYS111 (4.39-IC2)							✓			✓
21	ASP115 (IC2)--LYS111(IC2)						✓				
22	ASP115-LYS49 (IC2-IC1)								✓		
23	GLU46-LYS45 (IC1-IC1)		✓								
24	GLU46-ARG48 (IC1-IC1)										✓
25	GLU46-LYS53 (IC1-2.41)										✓
26	GLU46-LYS213 (IC1-6.32)				✓						
27	GLU46-ARG217 (IC1-6.36)			✓							
28	ASP115-ARG107 (IC2 - 3.52)										✓
29	ASP201-ARG193 IC3-5.73							✓			
30	ASP201-ARG190 IC3-5.70								✓		✓

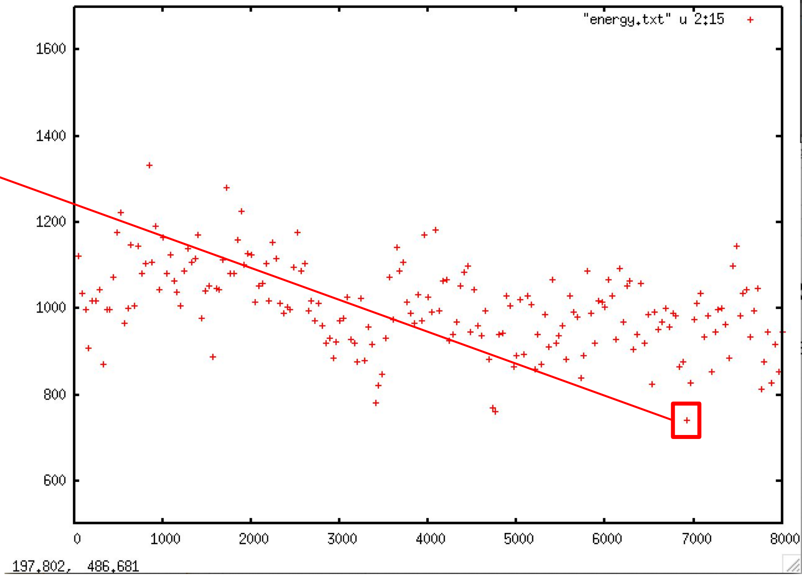
Protein_Energy 03Ci_GCR1- final 20ns (for a total of 60ns)

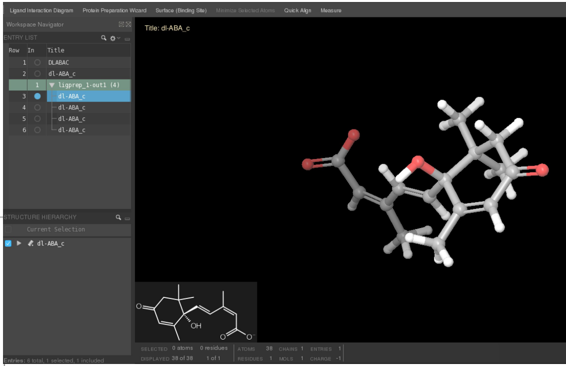
ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW	BOUNDARY	MISC	KINETIC	TOTAL
1	2	3	4	5	6	7	8	9 = 0	10 = 0	11 = 0	12

TEMP	TOTAL2	TOTAL3	TEMPAVG
13 = 0	14	15	16

```
ENERGY:    6840      1483.2297      2278.1369      1217.4633         8.8070          -36
77.1293      -474.2020       0.0000         0.0000         0.0000                836.3056
        0.0000       863.0538       864.1580        0.0000
ENERGY:    6880      1545.6749      2244.1252      1235.7382         9.0984          -36
53.7482      -529.1140       0.0000         0.0000         0.0000                851.7746
        0.0000       879.4292       877.0654        0.0000
ENERGY:    6920      1432.1855      2251.3573      1235.2047         9.2194          -36
97.5373      -520.3953       0.0000         0.0000         0.0000                710.0343
        0.0000       736.0399       740.0076        0.0000
ENERGY:    6960      1486.8427      2205.0663      1186.7286         9.7359          -36
05.7423      -481.5155       0.0000         0.0000         0.0000                801.1157
        0.0000       828.1909       827.8995        0.0000
ENERGY:    7000      1511.2239      2231.3902      1215.3981         9.5319          -35
34.7335      -486.1753       0.0000         0.0000         0.0000                946.6351
        0.0000       973.1079       975.0938        0.0000
ENERGY:    7040      1550.8034      2215.5868      1222.1893         9.4801          -35
04.8053      -504.9068       0.0000         0.0000         0.0000                988.3475
        0.0000      1016.3801      1012.3924        0.0000
ENERGY:    7080      1498.7123      2240.0066      1238.3976        10.5204          -35
08.2504      -472.6444       0.0000         0.0000         0.0000               1006.7421
        0.0000      1033.5664      1034.3591        0.0000
ENERGY:    7120      1461.6218      2260.0809      1195.3123         9.1059          -35
36.8360      -480.8973       0.0000         0.0000         0.0000                908.3876
        0.0000       935.5020       935.1574        0.0000
ENERGY:    7160      1522.7308      2226.0508      1207.7865        11.6127          -35
61.3073      -450.4778       0.0000         0.0000         0.0000                956.3956
        0.0000       983.0889       984.3451        0.0000
ENERGY:    7200      1493.2619      2220.4058      1229.8103         9.2505          -36
54.5596      -471.2731       0.0000         0.0000         0.0000                826.8958
        0.0000       853.9214       853.8530        0.0000
ENERGY:    7240      1488.0941      2267.6604      1203.0971         8.7559          -35
68.4987      -478.6719       0.0000         0.0000         0.0000                920.4370
        0.0000       947.9171       946.1485        0.0000
ENERGY:    7280      1524.4276      2205.6783      1200.7308         8.4043          -35
07.1918      -458.5969       0.0000         0.0000         0.0000                973.4523
        0.0000      1001.8985       996.6176        0.0000
ENERGY:    7320      1434.1980      2262.1416      1242.3688         9.0956          -35
31.7987      -443.9042       0.0000         0.0000         0.0000                972.1012
        0.0000       998.7036      1000.6668        0.0000
ENERGY:    7360      1506.7970      2226.9612      1192.3078        12.0465          -35
52.1912      -446.8179       0.0000         0.0000         0.0000                939.1034
        0.0000       966.9035       964.2529        0.0000
ENERGY:    7400      1482.3809      2232.4843      1223.6003         9.2942          -35
57.4251      -533.8377       0.0000         0.0000         0.0000                856.4969
        0.0000       883.1959       884.8402        0.0000
ENERGY:    7440      1456.4151      2290.2810      1235.6957        10.7488          -34
58.0175      -464.0699       0.0000         0.0000         0.0000               1071.0532
        0.0000      1098.4218      1097.4519        0.0000
@
@
                                                                  173,1         92%
```

TOTAL 3

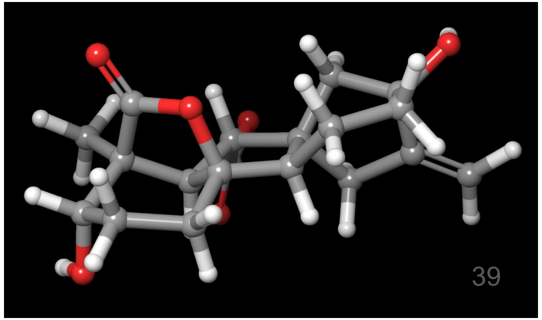




Title: dl-ABA_c

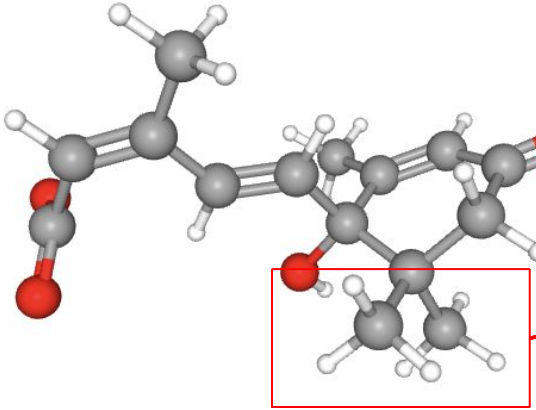
Row	In	Title
1	○	DLABAC
2	○	dl-ABA_c
	1	ligprep_1-out1 (4)
3	●	dl-ABA_c
4	○	dl-ABA_c
5	○	dl-ABA_c
6	○	dl-ABA_c

SELECTED 0 atoms 0 residues
DISPLAYED 38 of 38 1 of 1
ATOMS 38 CHAINS 1 ENTRIES 1
RESIDUES 1 MOLS 1 CHARGE -1
Entries: 6 total, 1 selected, 1 included

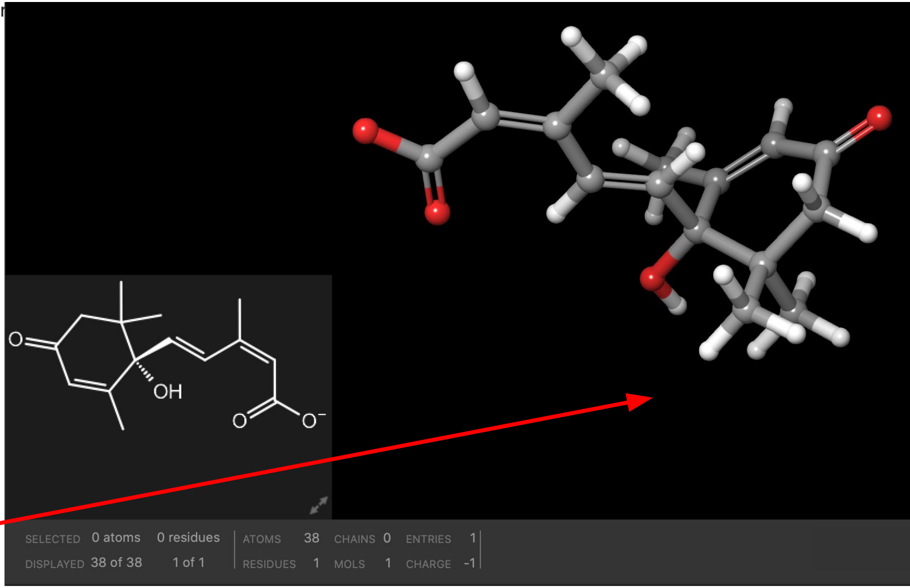


Ligands: ABA

(+)-abscisic acid is the naturally occurring (1'S)-(+) enantiomer of abscisic acid. It is an important sesquiterpenoid plant hormone which acts as a regulator of plant responses to environmental stresses such as drought and cold. It has a role as a plant hormone and a plant metabolite. It is a conjugate acid of a (+)-abscisate. It is an enantiomer of a (-)-abscisic acid.

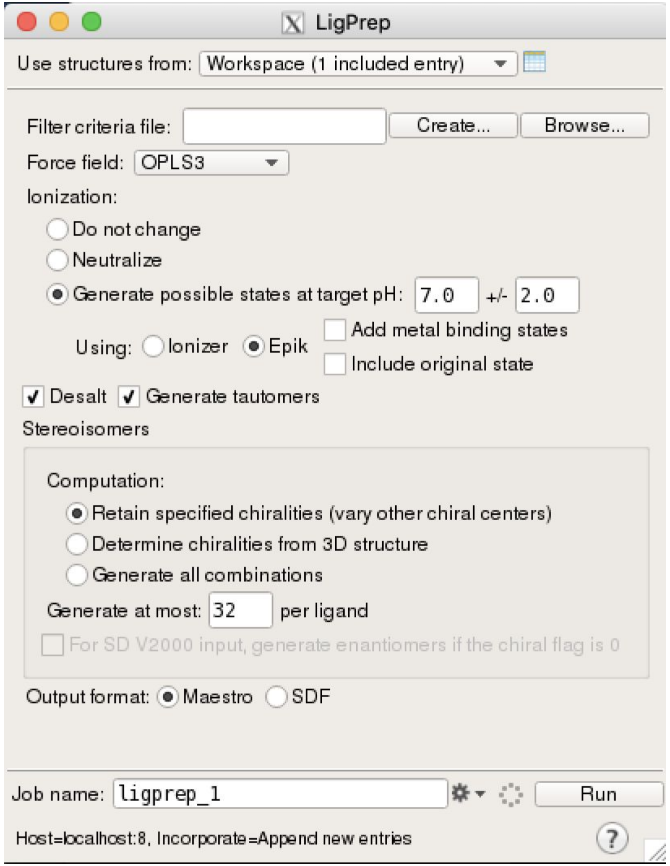


Downloaded from ccdc.cam.ac.uk/



SELECTED 0 atoms 0 residues
DISPLAYED 38 of 38 1 of 1
ATOMS 38 CHAINS 0 ENTRIES 1
RESIDUES 1 MOLS 1 CHARGE -1

Ligands: From n_ABA to c_ABA



Use structures from: Workspace (1 included entry)

Filter criteria file: ☐

Force field: OPLS3

Ionization:
- ○ Do not change
- ○ Neutralize
- ● Generate possible states at target pH: 7.0 +/- 2.0

Using: ○ Ionizer ● Epik

☐ Add metal binding states

☐ Include original state

☑ Desalt ☑ Generate tautomers

Stereoisomers

Computation:
- ● Retain specified chiralities (vary other chiral centers)
- ○ Determine chiralities from 3D structure
- ○ Generate all combinations

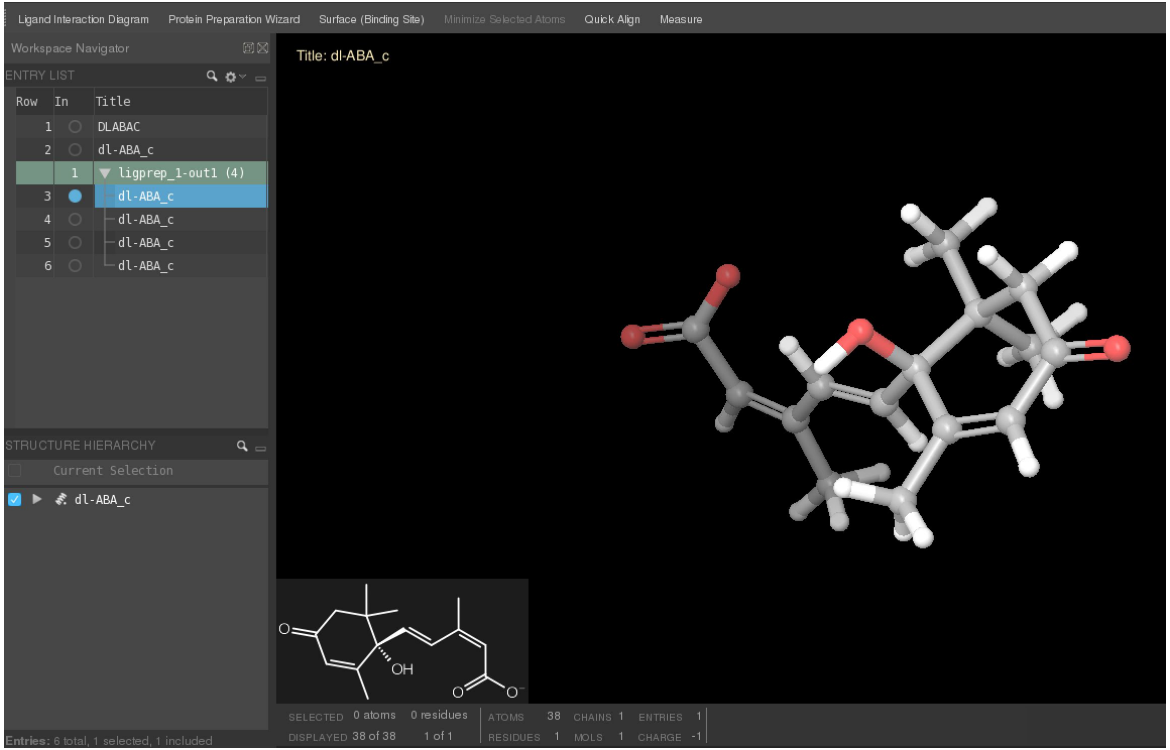
Generate at most: 32 per ligand

☐ For SD V2000 input, generate enantiomers if the chiral flag is 0

Output format: ● Maestro ○ SDF

Job name: ligprep_1

Host=localhost:8, Incorporate=Append new entries



Title: dl-ABA_c

Row	In	Title
1	○	DLABAC
2	○	dl-ABA_c
1		▼ ligprep_1-out1 (4)
3	●	dl-ABA_c
4	○	dl-ABA_c
5	○	dl-ABA_c
6	○	dl-ABA_c

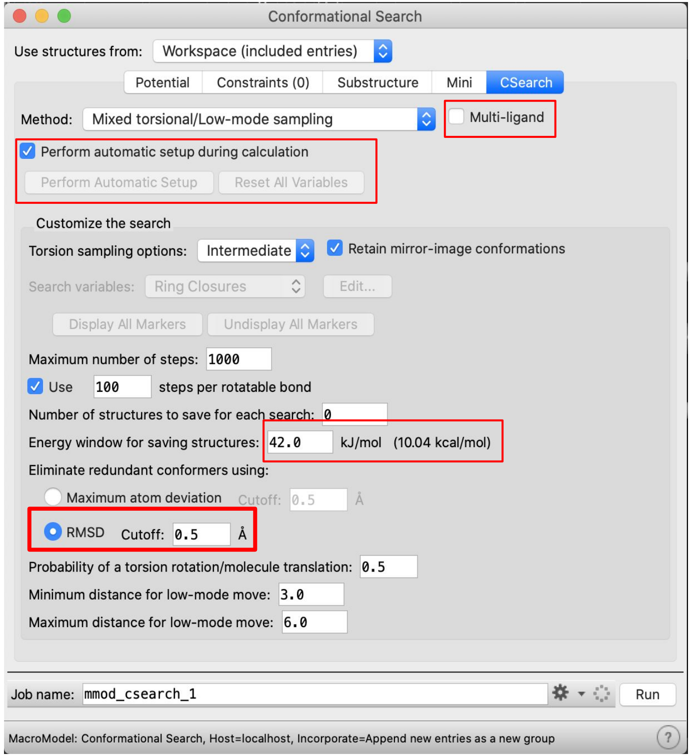
☑ ▶ dl-ABA_c

Entries: 6 total, 1 selected, 1 included

SELECTED 0 atoms 0 residues ATOMS 38 CHAINS 1 ENTRIES 1

DISPLAYED 38 of 38 1 of 1 RESIDUES 1 MOLS 1 CHARGE -1

Ligands: From n_ABA to c_ABA



Conformational Search

Use structures from: Workspace (included entries)

Method: Mixed torsional/Low-mode sampling ☐ Multi-ligand

☑ Perform automatic setup during calculation

Customize the search

Torsion sampling options: Intermediate ☑ Retain mirror-image conformations

Search variables: Ring Closures Edit...

Maximum number of steps: 1000

☑ Use 100 steps per rotatable bond

Number of structures to save for each search: 0

Energy window for saving structures: 42.0 kJ/mol (10.04 kcal/mol)

Eliminate redundant conformers using:

○ Maximum atom deviation Cutoff: 0.5 Å

● RMSD Cutoff: 0.5 Å

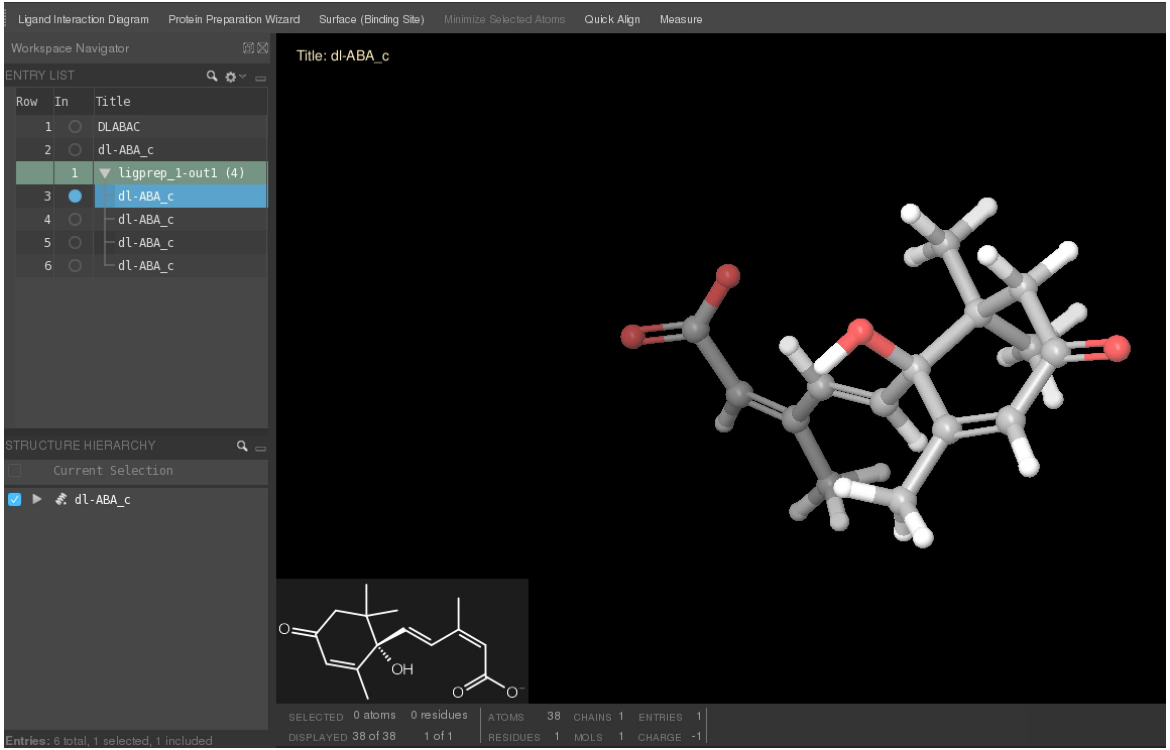
Probability of a torsion rotation/molecule translation: 0.5

Minimum distance for low-mode move: 3.0

Maximum distance for low-mode move: 6.0

Job name: mmod_csearch_1

MacroModel: Conformational Search, Host=localhost, Incorporate=Append new entries as a new group



Row	In	Title
1	○	DLABAC
2	○	dl-ABA_c
	1	▼ ligprep_1-out1 (4)
3	●	dl-ABA_c
4	○	dl-ABA_c
5	○	dl-ABA_c
6	○	dl-ABA_c

Current Selection

☑ ▶ dl-ABA_c

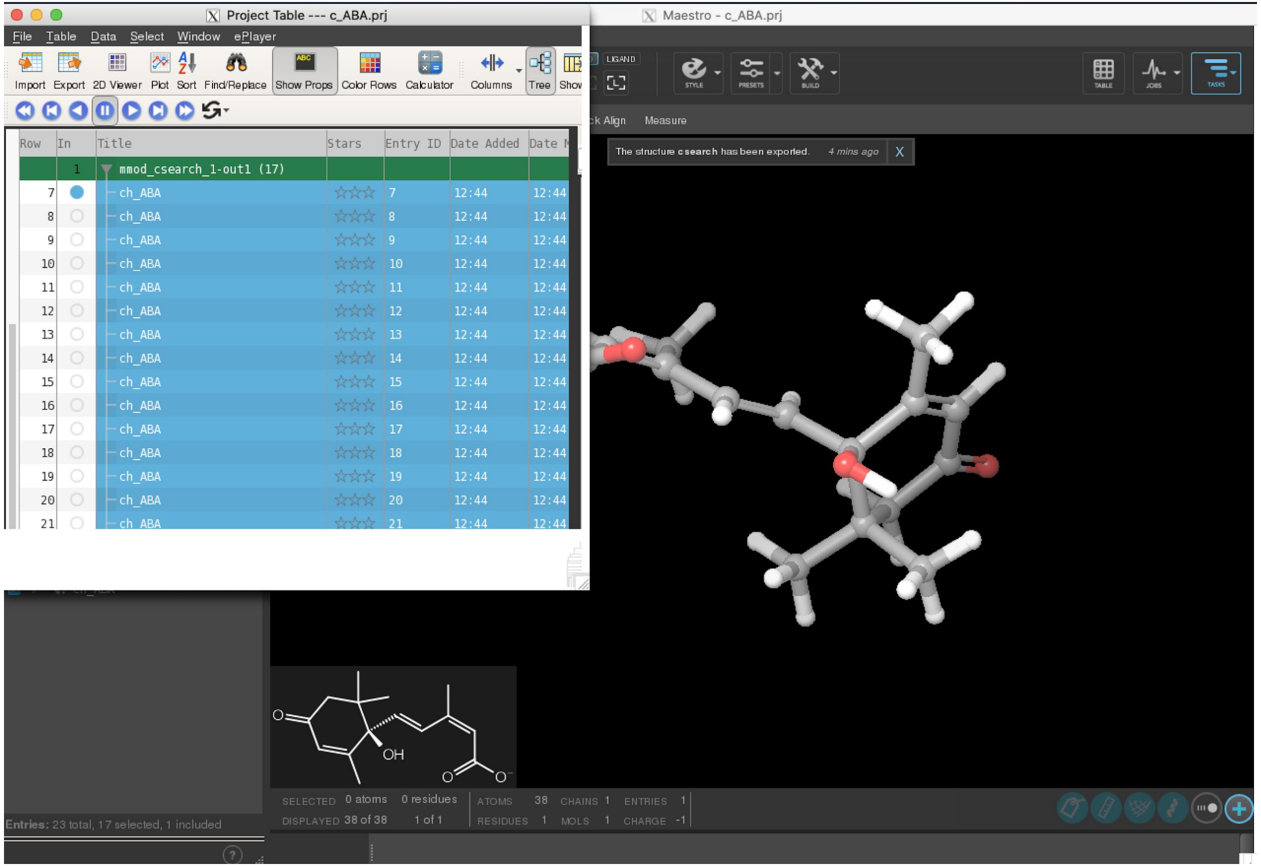
Title: dl-ABA_c

SELECTED 0 atoms 0 residues
DISPLAYED 38 of 38 1 of 1

ATOMS 38 CHAINS 1 ENTRIES 1
RESIDUES 1 MOLS 1 CHARGE -1

Entries: 6 total, 1 selected, 1 included

Ligands: ABA_conformers



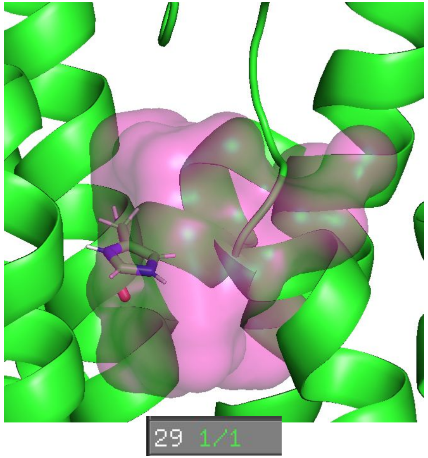
Row	In	Title	Stars	Entry ID	Date Added	Date M
	1	mmod_csearch_1-out1 (17)				
7	●	ch_ABA	☆☆☆	7	12:44	12:44
8	○	ch_ABA	☆☆☆	8	12:44	12:44
9	○	ch_ABA	☆☆☆	9	12:44	12:44
10	○	ch_ABA	☆☆☆	10	12:44	12:44
11	○	ch_ABA	☆☆☆	11	12:44	12:44
12	○	ch_ABA	☆☆☆	12	12:44	12:44
13	○	ch_ABA	☆☆☆	13	12:44	12:44
14	○	ch_ABA	☆☆☆	14	12:44	12:44
15	○	ch_ABA	☆☆☆	15	12:44	12:44
16	○	ch_ABA	☆☆☆	16	12:44	12:44
17	○	ch_ABA	☆☆☆	17	12:44	12:44
18	○	ch_ABA	☆☆☆	18	12:44	12:44
19	○	ch_ABA	☆☆☆	19	12:44	12:44
20	○	ch_ABA	☆☆☆	20	12:44	12:44
21	○	ch_ABA	☆☆☆	21	12:44	12:44

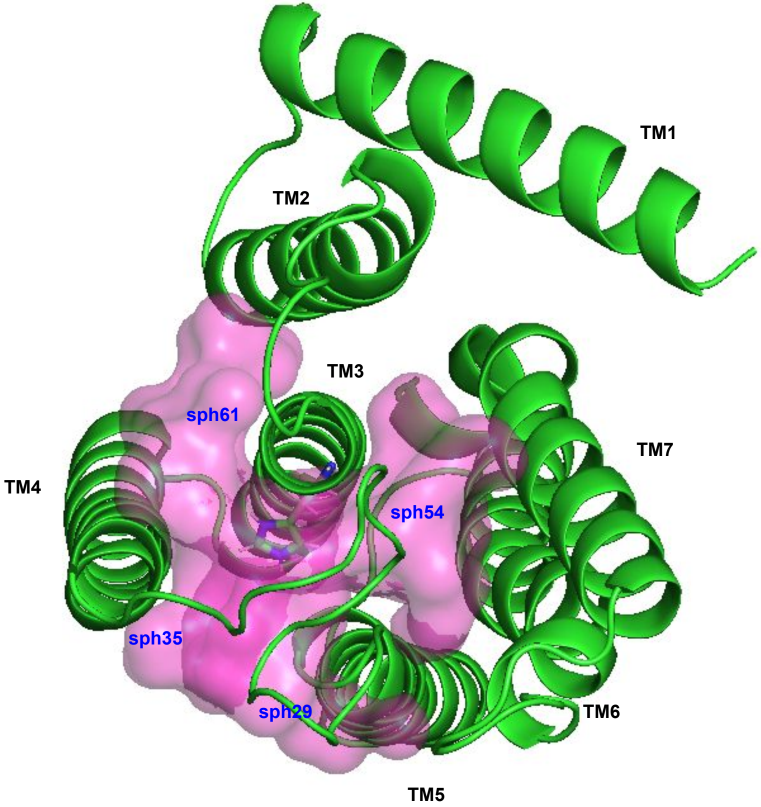
The structure csearch has been exported. 4 mins ago X

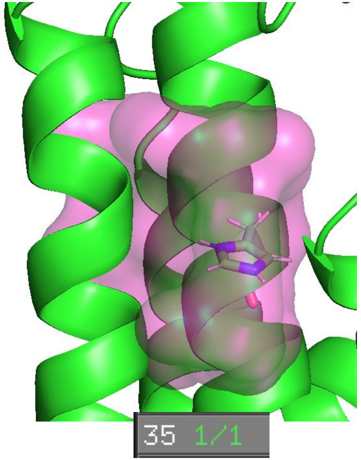
SELECTED 0 atoms 0 residues
DISPLAYED 38 of 38 1 of 1
ATOMS 38
RESIDUES 1
CHAINS 1
MOLS 1
ENTRIES 1
CHARGE -1

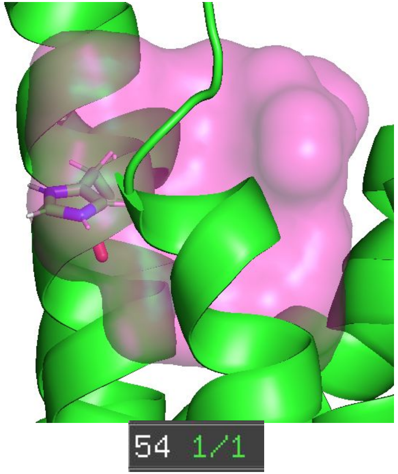
Entries: 23 total, 17 selected, 1 included

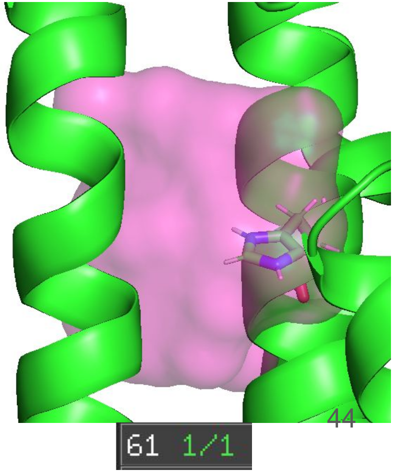
Spheres (29,35,54,61) around protonated Histidine, HSP, on 03Ci_GCR1



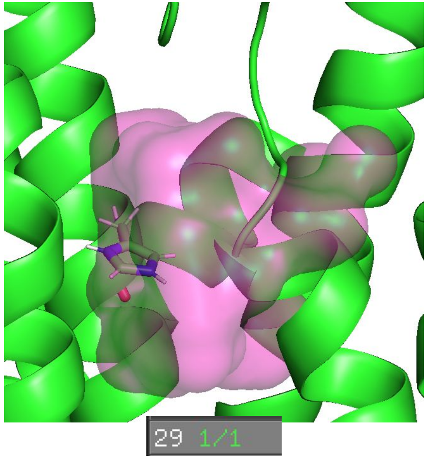


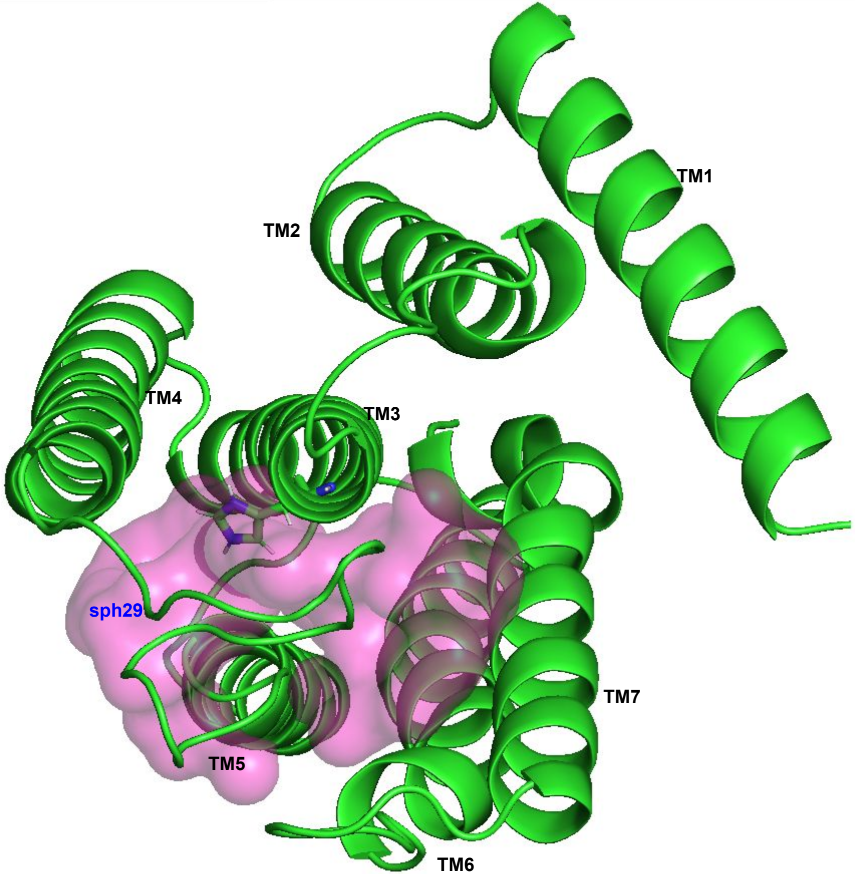


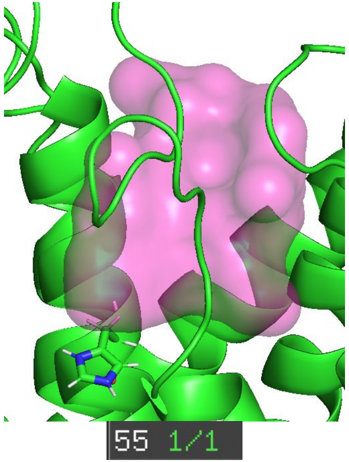




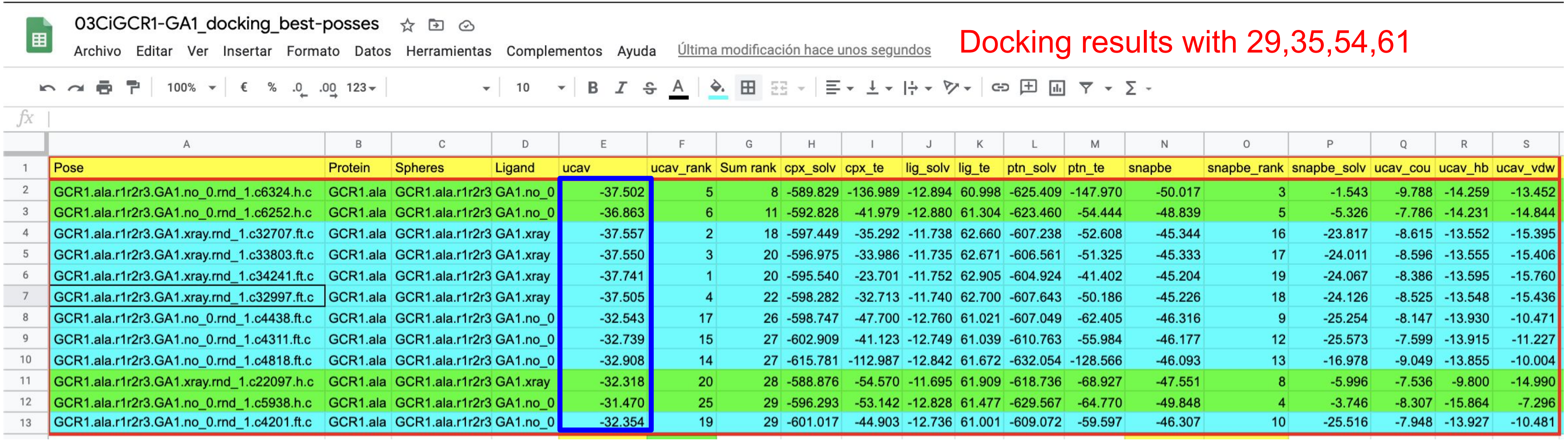
Spheres (29,55) around protonated Histidine, HSP, on 03Ci_GCR1







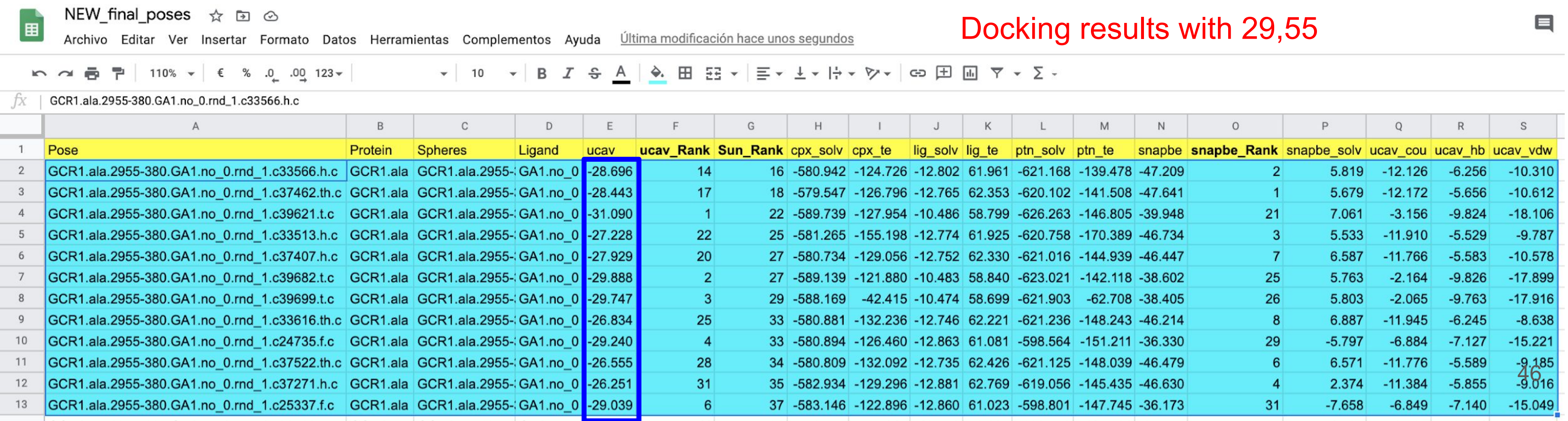
Docking results with 29,35,54,61



03CiGCR1-GA1_docking_best-posses

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Pose	Protein	Spheres	Ligand	ucav	ucav_rank	Sum rank	cpx_solv	cpx_te	lig_solv	lig_te	ptn_solv	ptn_te	snapbe	snapbe_rank	snapbe_solv	ucav_cou	ucav_hb	ucav_vdw
2	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c6324.h.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-37.502	5	8	-589.829	-136.989	-12.894	60.998	-625.409	-147.970	-50.017	3	-1.543	-9.788	-14.259	-13.452
3	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c6252.h.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-36.863	6	11	-592.828	-41.979	-12.880	61.304	-623.460	-54.444	-48.839	5	-5.326	-7.786	-14.231	-14.844
4	GCR1.ala.r1r2r3.GA1.xray.rnd_1.c32707.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.xray	-37.557	2	18	-597.449	-35.292	-11.738	62.660	-607.238	-52.608	-45.344	16	-23.817	-8.615	-13.552	-15.395
5	GCR1.ala.r1r2r3.GA1.xray.rnd_1.c33803.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.xray	-37.550	3	20	-596.975	-33.986	-11.735	62.671	-606.561	-51.325	-45.333	17	-24.011	-8.596	-13.555	-15.406
6	GCR1.ala.r1r2r3.GA1.xray.rnd_1.c34241.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.xray	-37.741	1	20	-595.540	-23.701	-11.752	62.905	-604.924	-41.402	-45.204	19	-24.067	-8.386	-13.595	-15.760
7	GCR1.ala.r1r2r3.GA1.xray.rnd_1.c32997.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.xray	-37.505	4	22	-598.282	-32.713	-11.740	62.700	-607.643	-50.186	-45.226	18	-24.126	-8.525	-13.548	-15.436
8	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c4438.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-32.543	17	26	-598.747	-47.700	-12.760	61.021	-607.049	-62.405	-46.316	9	-25.254	-8.147	-13.930	-10.471
9	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c4311.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-32.739	15	27	-602.909	-41.123	-12.749	61.039	-610.763	-55.984	-46.177	12	-25.573	-7.599	-13.915	-11.227
10	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c4818.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-32.908	14	27	-615.781	-112.987	-12.842	61.672	-632.054	-128.566	-46.093	13	-16.978	-9.049	-13.855	-10.004
11	GCR1.ala.r1r2r3.GA1.xray.rnd_1.c22097.h.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.xray	-32.318	20	28	-588.876	-54.570	-11.695	61.909	-618.736	-68.927	-47.551	8	-5.996	-7.536	-9.800	-14.990
12	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c5938.h.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-31.470	25	29	-596.293	-53.142	-12.828	61.477	-629.567	-64.770	-49.848	4	-3.746	-8.307	-15.864	-7.296
13	GCR1.ala.r1r2r3.GA1.no_0.rnd_1.c4201.ft.c	GCR1.ala	GCR1.ala.r1r2r3	GA1.no_0	-32.354	19	29	-601.017	-44.903	-12.736	61.001	-609.072	-59.597	-46.307	10	-25.516	-7.948	-13.927	-10.481

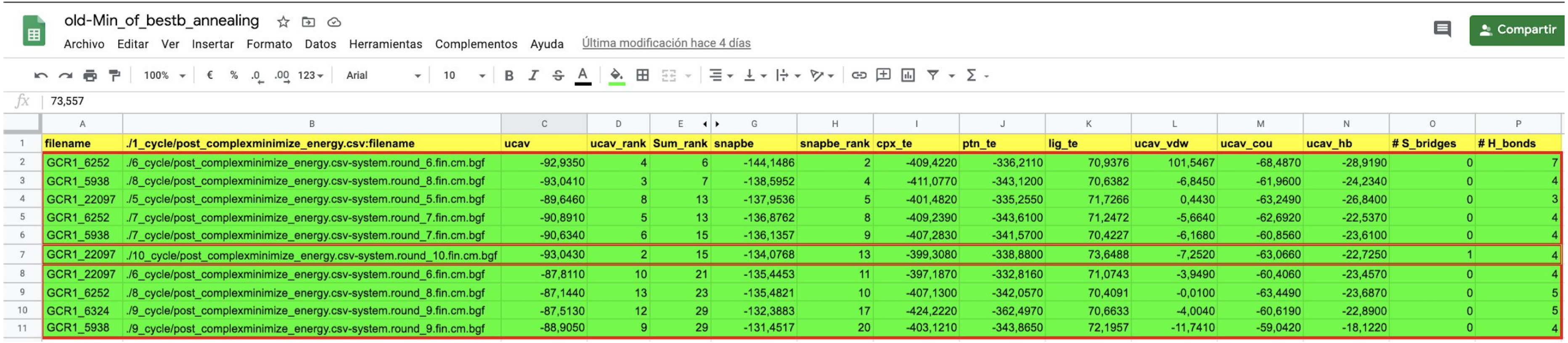
Docking results with 29,55



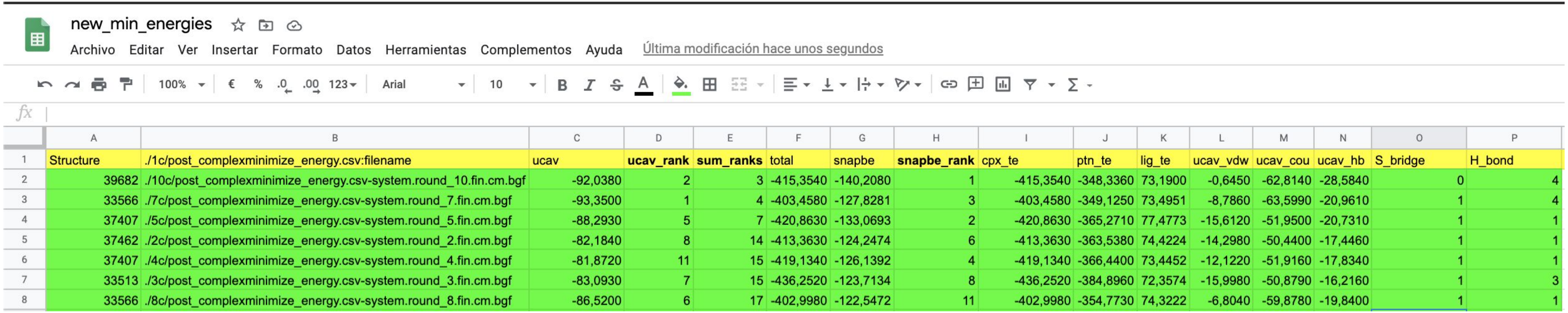
NEW_final_poses

fx GCR1.ala.2955-380.GA1.no_0.rnd_1.c33566.h.c

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Pose	Protein	Spheres	Ligand	ucav	**ucav_Rank**	**Sun_Rank**	cpx_solv	cpx_te	lig_solv	lig_te	ptn_solv	ptn_te	snapbe	**snapbe_Rank**	snapbe_solv	ucav_cou	ucav_hb	ucav_vdw
2	GCR1.ala.2955-380.GA1.no_0.rnd_1.c33566.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-28.696	14	16	-580.942	-124.726	-12.802	61.961	-621.168	-139.478	-47.209	2	5.819	-12.126	-6.256	-10.310
3	GCR1.ala.2955-380.GA1.no_0.rnd_1.c37462.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-28.443	17	18	-579.547	-126.796	-12.765	62.353	-620.102	-141.508	-47.641	1	5.679	-12.172	-5.656	-10.612
4	GCR1.ala.2955-380.GA1.no_0.rnd_1.c39621.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-31.090	1	22	-589.739	-127.954	-10.486	58.799	-626.263	-146.805	-39.948	21	7.061	-3.156	-9.824	-18.106
5	GCR1.ala.2955-380.GA1.no_0.rnd_1.c33513.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-27.228	22	25	-581.265	-155.198	-12.774	61.925	-620.758	-170.389	-46.734	3	5.533	-11.910	-5.529	-9.787
6	GCR1.ala.2955-380.GA1.no_0.rnd_1.c37407.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-27.929	20	27	-580.734	-129.056	-12.752	62.330	-621.016	-144.939	-46.447	7	6.587	-11.766	-5.583	-10.578
7	GCR1.ala.2955-380.GA1.no_0.rnd_1.c39682.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.888	2	27	-589.139	-121.880	-10.483	58.840	-623.021	-142.118	-38.602	25	5.763	-2.164	-9.826	-17.899
8	GCR1.ala.2955-380.GA1.no_0.rnd_1.c39699.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.747	3	29	-588.169	-42.415	-10.474	58.699	-621.903	-62.708	-38.405	26	5.803	-2.065	-9.763	-17.916
9	GCR1.ala.2955-380.GA1.no_0.rnd_1.c33616.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.834	25	33	-580.881	-132.236	-12.746	62.221	-621.236	-148.243	-46.214	8	6.887	-11.945	-6.245	-8.638
10	GCR1.ala.2955-380.GA1.no_0.rnd_1.c24735.f.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.240	4	33	-580.894	-126.460	-12.863	61.081	-598.564	-151.211	-36.330	29	-5.797	-6.884	-7.127	-15.221
11	GCR1.ala.2955-380.GA1.no_0.rnd_1.c37522.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.555	28	34	-580.809	-132.092	-12.735	62.426	-621.125	-148.039	-46.479	6	6.571	-11.776	-5.589	-9.185
12	GCR1.ala.2955-380.GA1.no_0.rnd_1.c37271.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.251	31	35	-582.934	-129.296	-12.881	62.769	-619.056	-145.435	-46.630	4	2.374	-11.384	-5.855	-9.016
13	GCR1.ala.2955-380.GA1.no_0.rnd_1.c25337.f.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.039	6	37	-583.146	-122.896	-12.860	61.023	-598.801	-147.745	-36.173	31	-7.658	-6.849	-7.140	-15.049

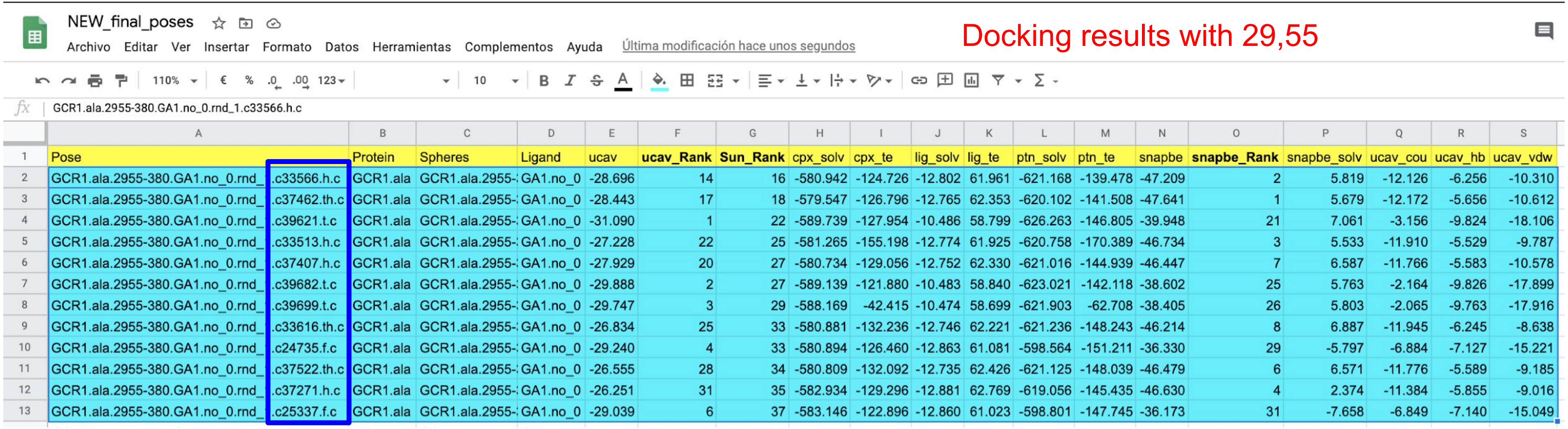


filename	./1_cycle/post_complexminimize_energy.csv:filename	ucav	ucav_rank	Sum_rank	snapbe	snapbe_rank	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	# S_bridges	# H_bonds
GCR1_6252	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-92,9350	4	6	-144,1486	2	-409,4220	-336,2110	70,9376	101,5467	-68,4870	-28,9190	0	7
GCR1_5938	./8_cycle/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-93,0410	3	7	-138,5952	4	-411,0770	-343,1200	70,6382	-6,8450	-61,9600	-24,2340	0	4
GCR1_22097	./5_cycle/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-89,6460	8	13	-137,9536	5	-401,4820	-335,2550	71,7266	0,4430	-63,2490	-26,8400	0	3
GCR1_6252	./7_cycle/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-90,8910	5	13	-136,8762	8	-409,2390	-343,6100	71,2472	-5,6640	-62,6920	-22,5370	0	4
GCR1_5938	./7_cycle/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-90,6340	6	15	-136,1357	9	-407,2830	-341,5700	70,4227	-6,1680	-60,8560	-23,6100	0	4
GCR1_22097	./10_cycle/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-93,0430	2	15	-134,0768	13	-399,3080	-338,8800	73,6488	-7,2520	-63,0660	-22,7250	1	4
GCR1_22097	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-87,8110	10	21	-135,4453	11	-397,1870	-332,8160	71,0743	-3,9490	-60,4060	-23,4570	0	4
GCR1_6252	./8_cycle/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-87,1440	13	23	-135,4821	10	-407,1300	-342,0570	70,4091	-0,0100	-63,4490	-23,6870	0	5
GCR1_6324	./9_cycle/post_complexminimize_energy.csv-system.round_9.fin.cm.bgf	-87,5130	12	29	-132,3883	17	-424,2220	-362,4970	70,6633	-4,0040	-60,6190	-22,8900	0	5
GCR1_5938	./9_cycle/post_complexminimize_energy.csv-system.round_9.fin.cm.bgf	-88,9050	9	29	-131,4517	20	-403,1210	-343,8650	72,1957	-11,7410	-59,0420	-18,1220	0	4



Structure	./1c/post_complexminimize_energy.csv:filename	ucav	ucav_rank	sum_ranks	total	snapbe	snapbe_rank	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	S_bridge	H_bond
39682	./10c/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-92,0380	2	3	-415,3540	-140,2080	1	-415,3540	-348,3360	73,1900	-0,6450	-62,8140	-28,5840	0	4
33566	./7c/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-93,3500	1	4	-403,4580	-127,8281	3	-403,4580	-349,1250	73,4951	-8,7860	-63,5990	-20,9610	1	4
37407	./5c/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-88,2930	5	7	-420,8630	-133,0693	2	-420,8630	-365,2710	77,4773	-15,6120	-51,9500	-20,7310	1	1
37462	./2c/post_complexminimize_energy.csv-system.round_2.fin.cm.bgf	-82,1840	8	14	-413,3630	-124,2474	6	-413,3630	-363,5380	74,4224	-14,2980	-50,4400	-17,4460	1	1
37407	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-81,8720	11	15	-419,1340	-126,1392	4	-419,1340	-366,4400	73,4452	-12,1220	-51,9160	-17,8340	1	1
33513	./3c/post_complexminimize_energy.csv-system.round_3.fin.cm.bgf	-83,0930	7	15	-436,2520	-123,7134	8	-436,2520	-384,8960	72,3574	-15,9980	-50,8790	-16,2160	1	3
33566	./8c/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-86,5200	6	17	-402,9980	-122,5472	11	-402,9980	-354,7730	74,3222	-6,8040	-59,8780	-19,8400	1	1

Docking results with 29,55



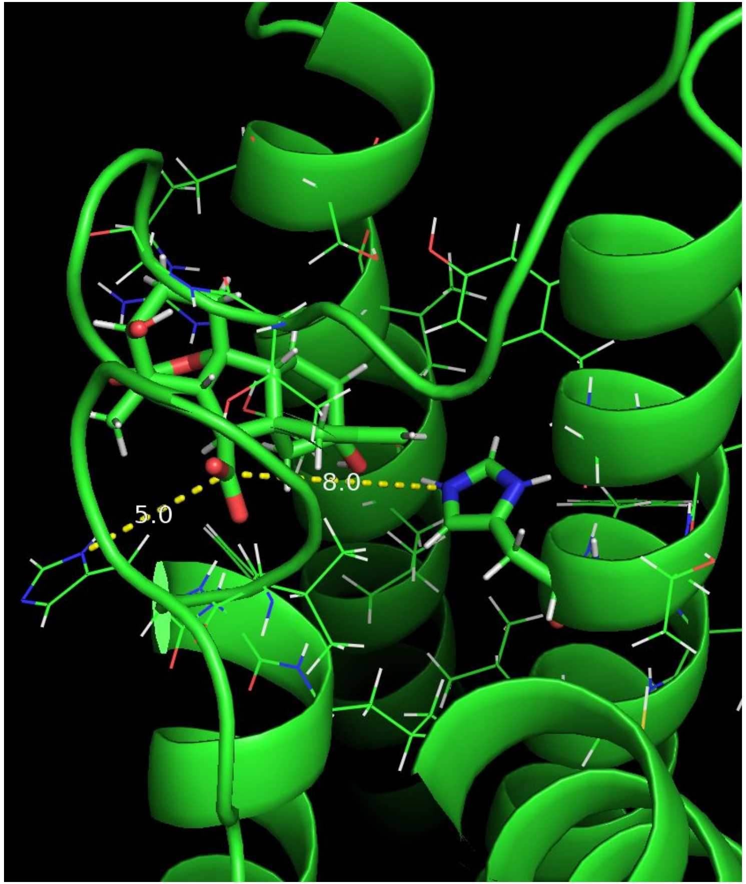
GCR1.ala.2955-380.GA1.no_0.rnd_1.c33566.h.c

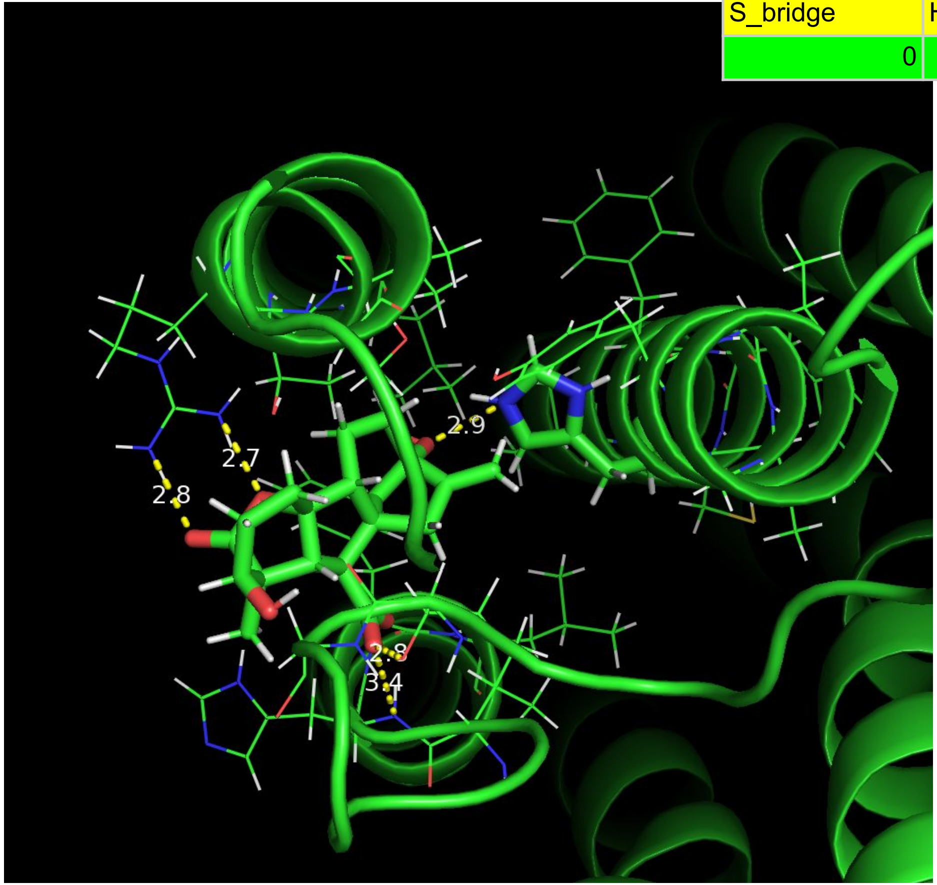
	Pose	Protein	Spheres	Ligand	ucav	**ucav_Rank**	**Sun_Rank**	cpx_solv	cpx_te	lig_solv	lig_te	ptn_solv	ptn_te	snapbe	**snapbe_Rank**	snapbe_solv	ucav_cou	ucav_hb	ucav_vdw
2	GCR1.ala.2955-380.GA1.no_0.rnd_ .c33566.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-28.696	14	16	-580.942	-124.726	-12.802	61.961	-621.168	-139.478	-47.209	2	5.819	-12.126	-6.256	-10.310
3	GCR1.ala.2955-380.GA1.no_0.rnd_ .c37462.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-28.443	17	18	-579.547	-126.796	-12.765	62.353	-620.102	-141.508	-47.641	1	5.679	-12.172	-5.656	-10.612
4	GCR1.ala.2955-380.GA1.no_0.rnd_ .c39621.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-31.090	1	22	-589.739	-127.954	-10.486	58.799	-626.263	-146.805	-39.948	21	7.061	-3.156	-9.824	-18.106
5	GCR1.ala.2955-380.GA1.no_0.rnd_ .c33513.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-27.228	22	25	-581.265	-155.198	-12.774	61.925	-620.758	-170.389	-46.734	3	5.533	-11.910	-5.529	-9.787
6	GCR1.ala.2955-380.GA1.no_0.rnd_ .c37407.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-27.929	20	27	-580.734	-129.056	-12.752	62.330	-621.016	-144.939	-46.447	7	6.587	-11.766	-5.583	-10.578
7	GCR1.ala.2955-380.GA1.no_0.rnd_ .c39682.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.888	2	27	-589.139	-121.880	-10.483	58.840	-623.021	-142.118	-38.602	25	5.763	-2.164	-9.826	-17.899
8	GCR1.ala.2955-380.GA1.no_0.rnd_ .c39699.t.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.747	3	29	-588.169	-42.415	-10.474	58.699	-621.903	-62.708	-38.405	26	5.803	-2.065	-9.763	-17.916
9	GCR1.ala.2955-380.GA1.no_0.rnd_ .c33616.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.834	25	33	-580.881	-132.236	-12.746	62.221	-621.236	-148.243	-46.214	8	6.887	-11.945	-6.245	-8.638
10	GCR1.ala.2955-380.GA1.no_0.rnd_ .c24735.f.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.240	4	33	-580.894	-126.460	-12.863	61.081	-598.564	-151.211	-36.330	29	-5.797	-6.884	-7.127	-15.221
11	GCR1.ala.2955-380.GA1.no_0.rnd_ .c37522.th.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.555	28	34	-580.809	-132.092	-12.735	62.426	-621.125	-148.039	-46.479	6	6.571	-11.776	-5.589	-9.185
12	GCR1.ala.2955-380.GA1.no_0.rnd_ .c37271.h.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-26.251	31	35	-582.934	-129.296	-12.881	62.769	-619.056	-145.435	-46.630	4	2.374	-11.384	-5.855	-9.016
13	GCR1.ala.2955-380.GA1.no_0.rnd_ .c25337.f.c	GCR1.ala	GCR1.ala.2955-	GA1.no_0	-29.039	6	37	-583.146	-122.896	-12.860	61.023	-598.801	-147.745	-36.173	31	-7.658	-6.849	-7.140	-15.049

Min_Docking 29,55

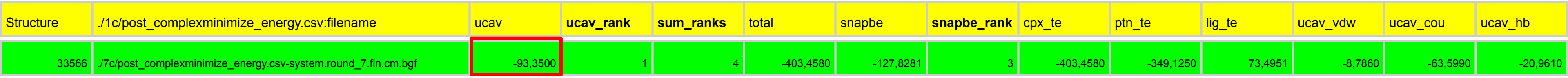
Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
39682	./10c/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-92,0380	2	3	-415,3540	-140,2080	1	-415,3540	-348,3360	73,1900	-0,6450	-62,8140	-28,5840
33566	./7c/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-93,3500	1	4	-403,4580	-127,8281	3	-403,4580	-349,1250	73,4951	-8,7860	-63,5990	-20,9610
37407	./5c/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-88,2930	5	7	-420,8630	-133,0693	2	-420,8630	-365,2710	77,4773	-15,6120	-51,9500	-20,7310
37462	./2c/post_complexminimize_energy.csv-system.round_2.fin.cm.bgf	-82,1840	8	14	-413,3630	-124,2474	6	-413,3630	-363,5380	74,4224	-14,2980	-50,4400	-17,4460
37407	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-81,8720	11	15	-419,1340	-126,1392	4	-419,1340	-366,4400	73,4452	-12,1220	-51,9160	-17,8340
33513	./3c/post_complexminimize_energy.csv-system.round_3.fin.cm.bgf	-83,0930	7	15	-436,2520	-123,7134	8	-436,2520	-384,8960	72,3574	-15,9980	-50,8790	-16,2160
33566	./8c/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-86,5200	6	17	-402,9980	-122,5472	11	-402,9980	-354,7730	74,3222	-6,8040	-59,8780	-19,8400
33566	./1c/post_complexminimize_energy.csv-system.round_1.fin.cm.bgf	-88,3140	4	19	-400,2000	-119,4056	15	-400,2000	-354,0740	73,2796	-10,9250	-61,1860	-16,2040
37407	./7c/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-80,6600	14	21	-420,0940	-124,0353	7	-420,0940	-368,8370	72,7783	-12,0440	-51,6080	-17,0110
33513	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-82,1080	10	24	-433,2580	-120,6882	14	-433,2580	-384,9140	72,3442	-14,3130	-51,0020	-16,7920

Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
39682	./10c/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-92,0380	2	3	-415,3540	-140,2080	1	-415,3540	-348,3360	73,1900	-0,6450	-62,8140	-28,5840



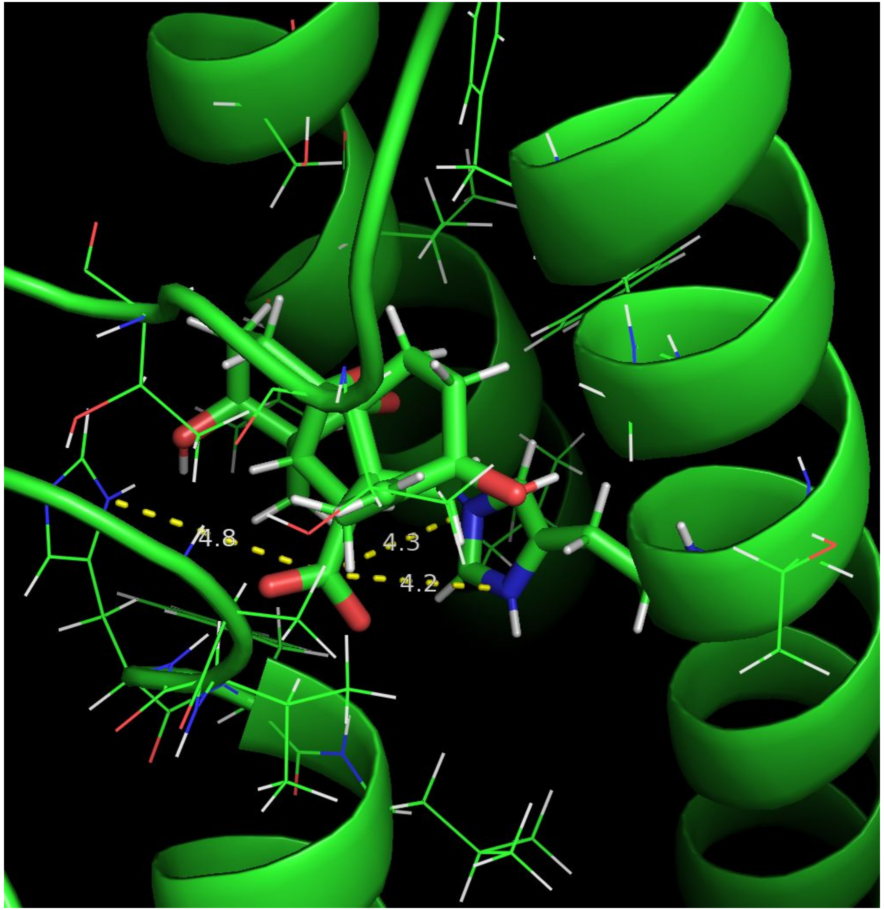


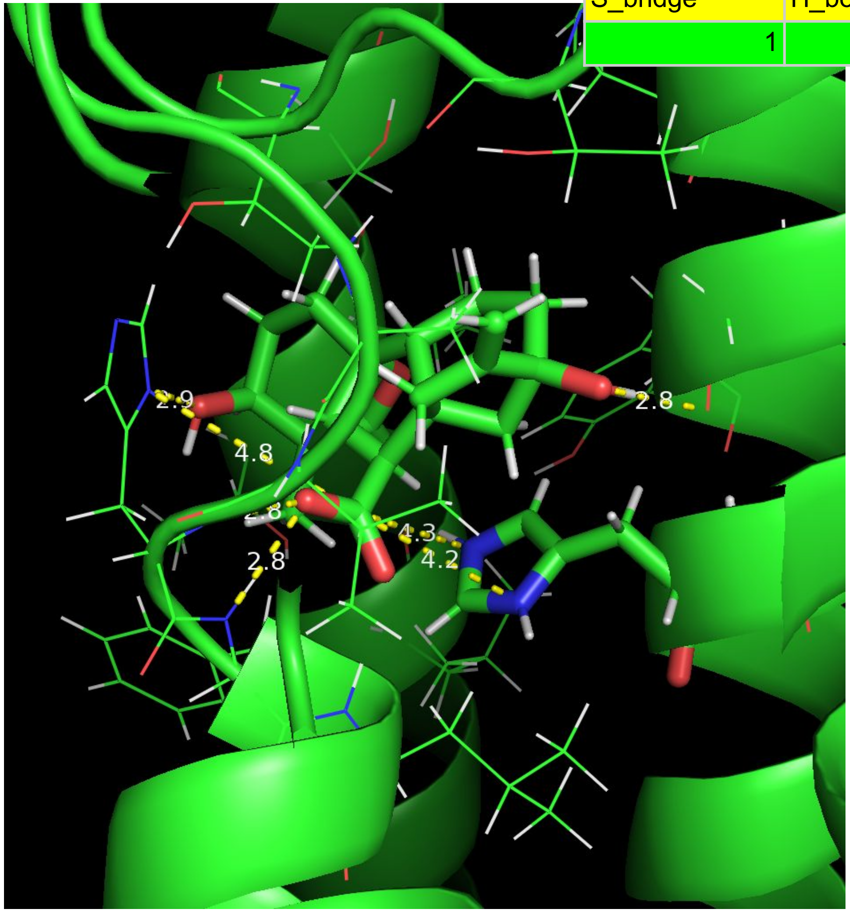
S_bridge	H_bond
0	4



Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
33566	./7c/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-93,3500	1	4	-403,4580	-127,8281	3	-403,4580	-349,1250	73,4951	-8,7860	-63,5990	-20,9610

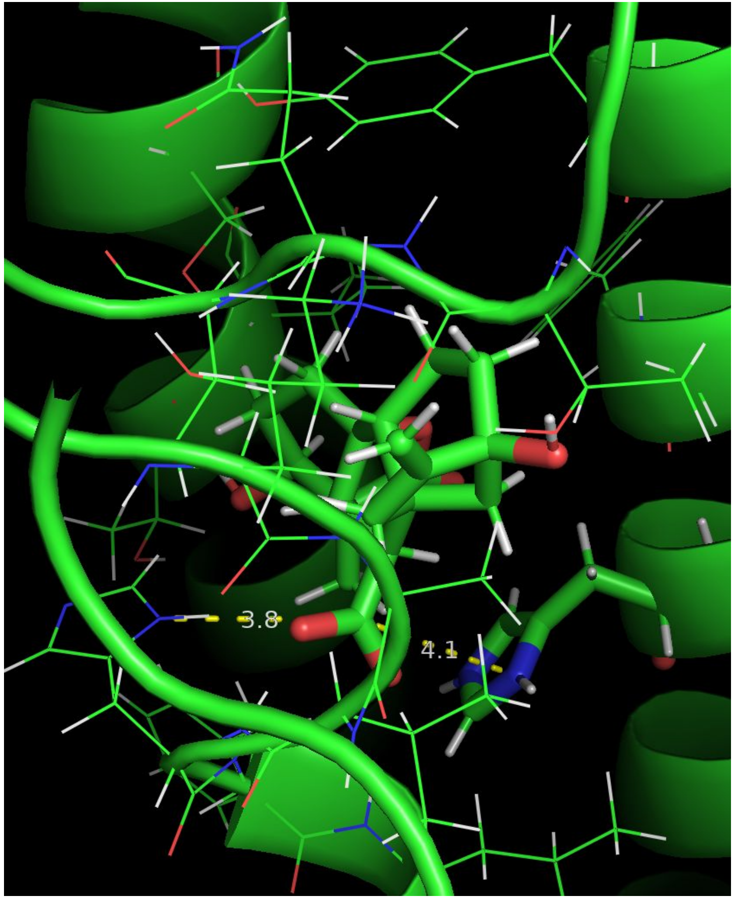
S_bridge	H_bond
1	4

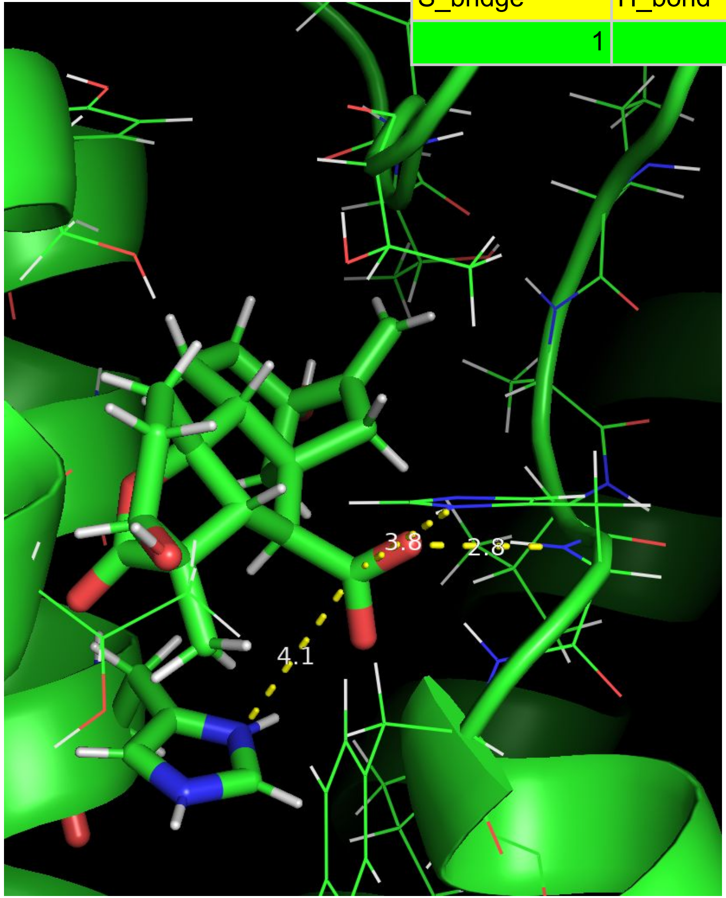




Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
37407	./5c/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-88,2930	5	7	-420,8630	-133,0693	2	-420,8630	-365,2710	77,4773	-15,6120	-51,9500	-20,7310

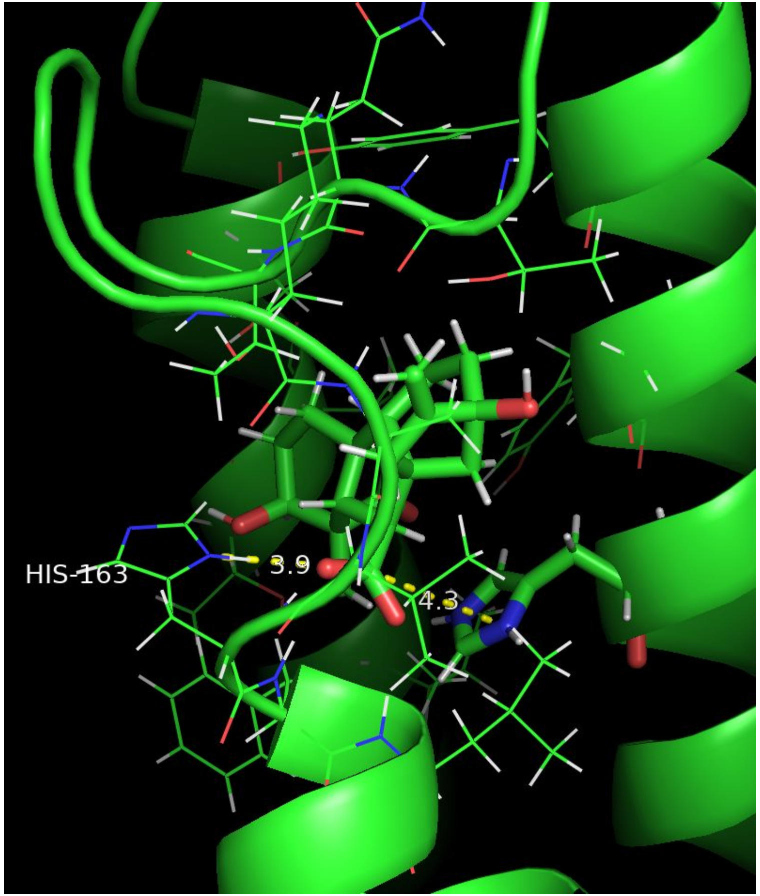
S_bridge	H_bond
1	1

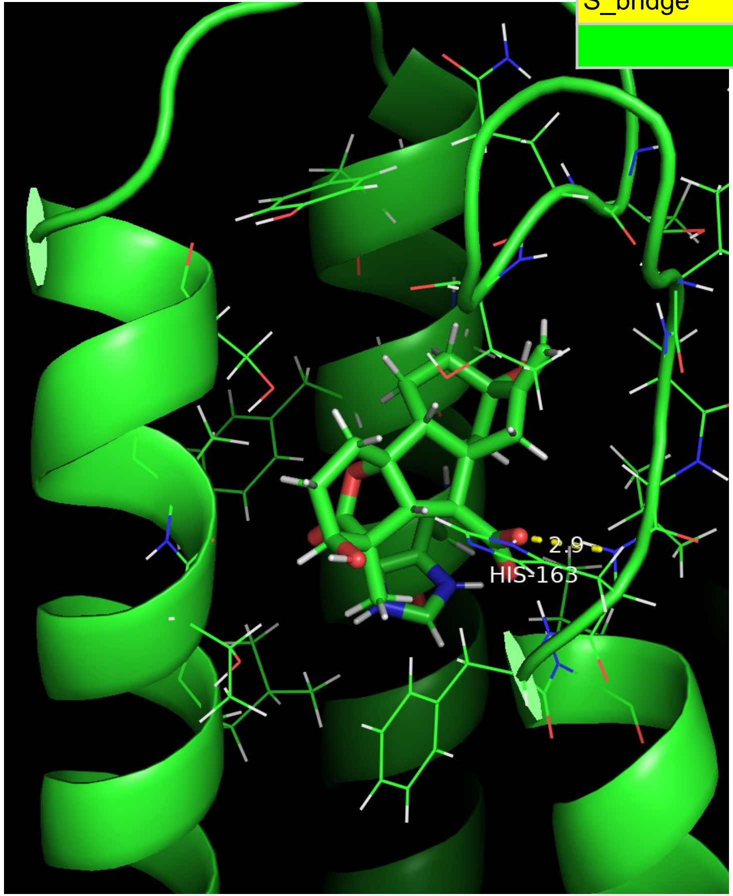




Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
37462	./2c/post_complexminimize_energy.csv-system.round_2.fin.cm.bgf	-82,1840	8	14	-413,3630	-124,2474	6	-413,3630	-363,5380	74,4224	-14,2980	-50,4400	-17,4460

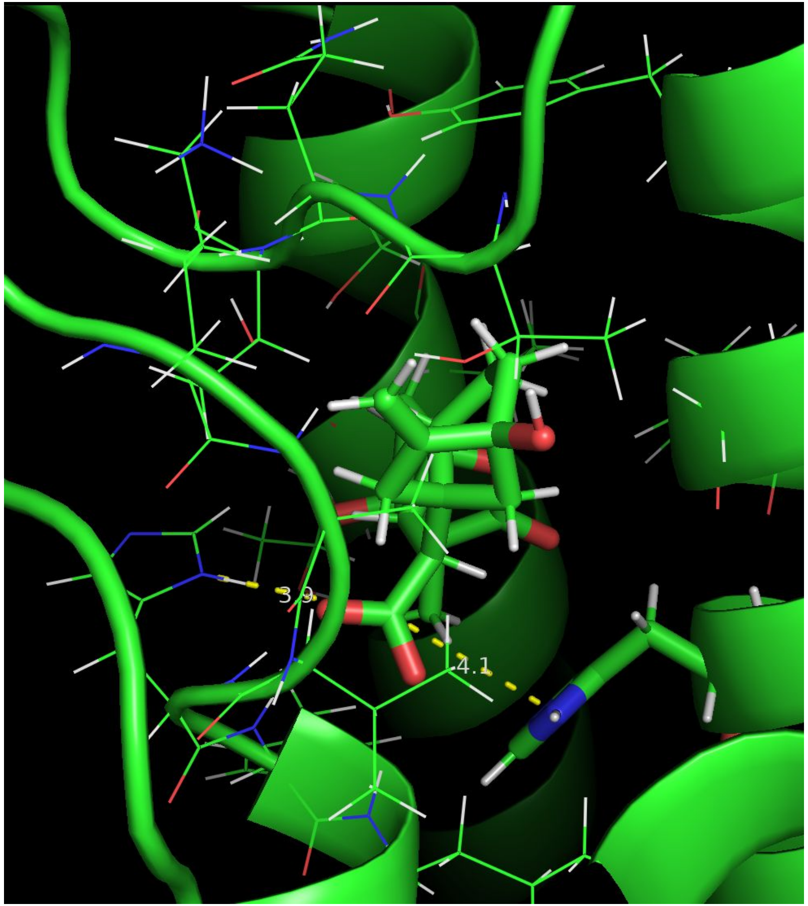
S_bridge	H_bond
1	1

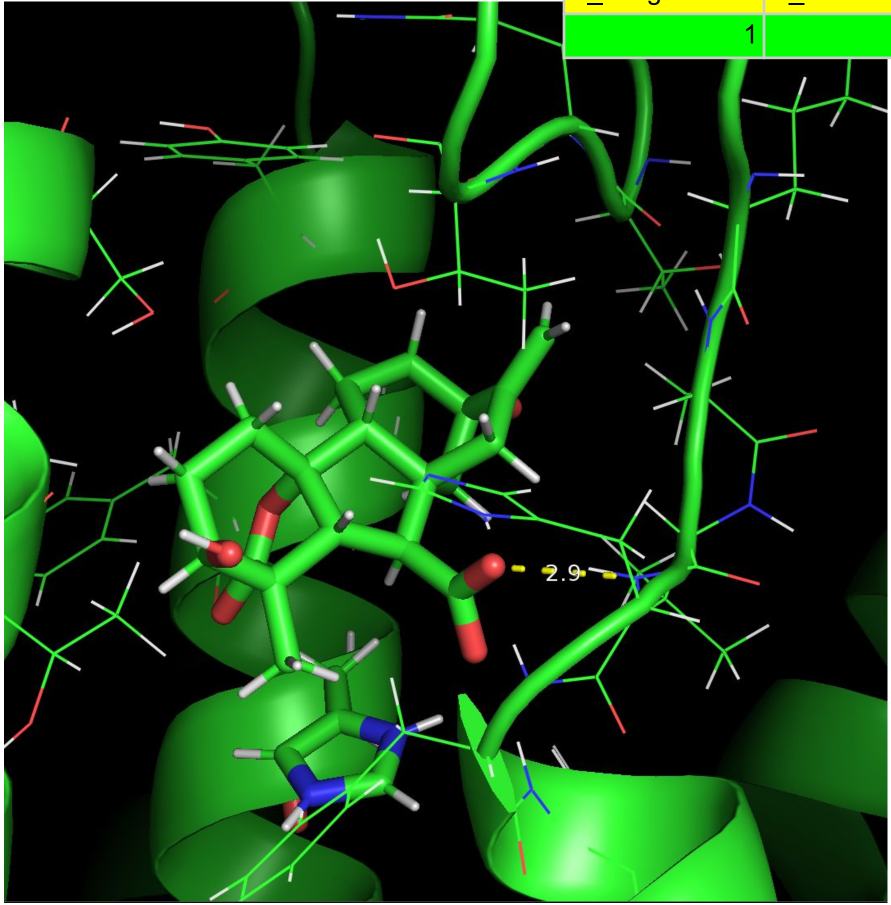




Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
37407	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-81,8720	11	15	-419,1340	-126,1392	4	-419,1340	-366,4400	73,4452	-12,1220	-51,9160	-17,8340

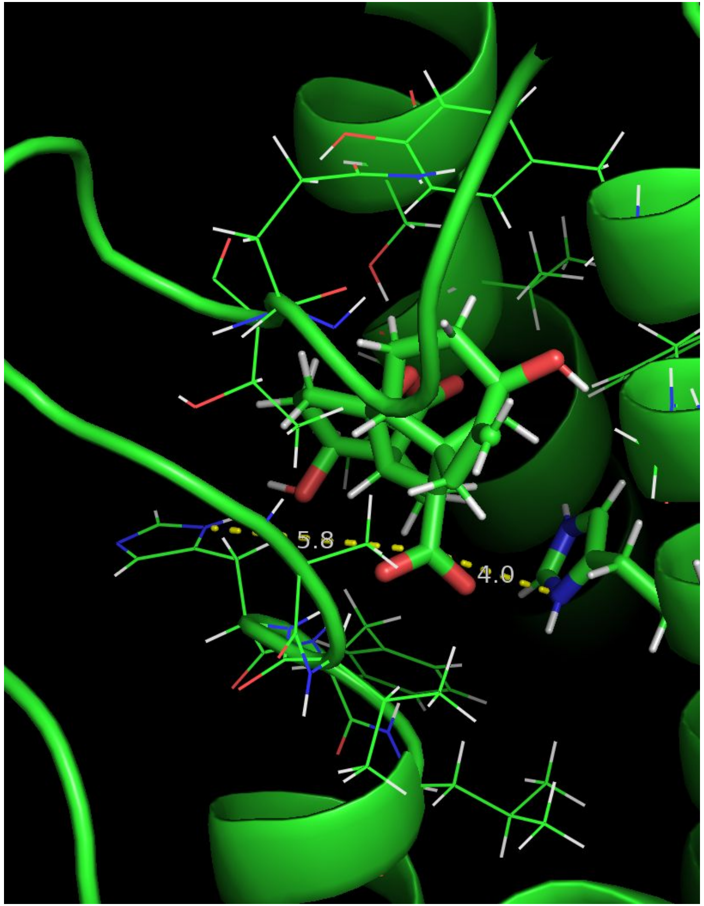
S_bridge	H_bond
1	1

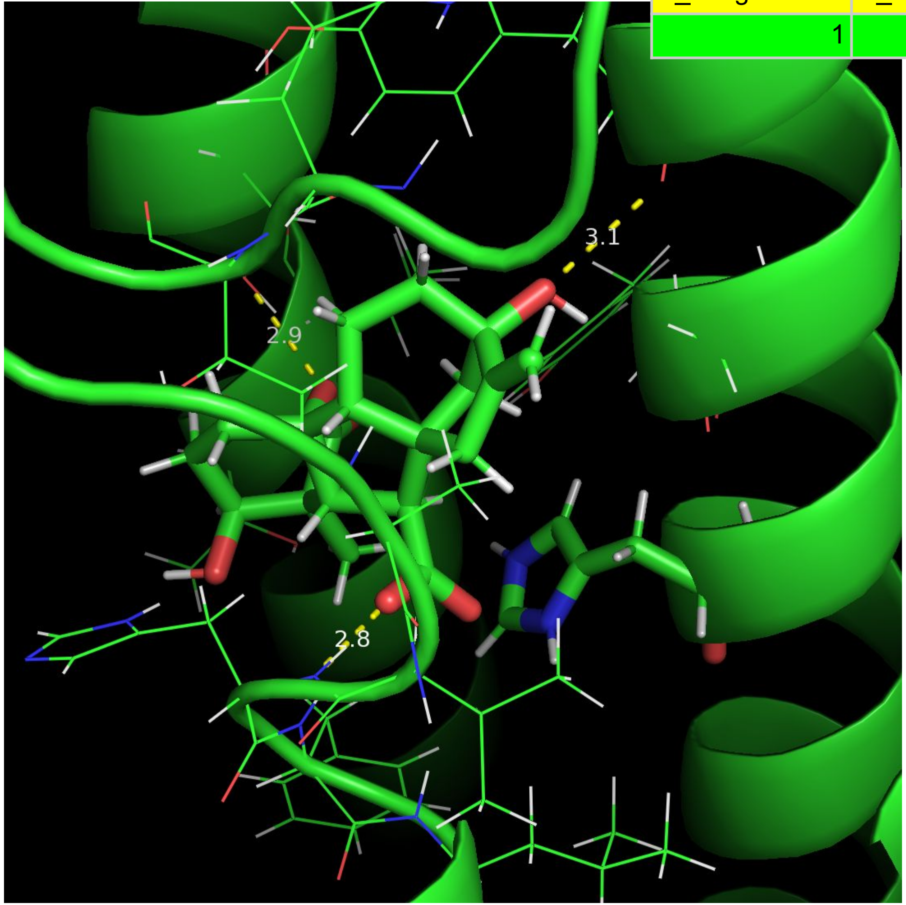




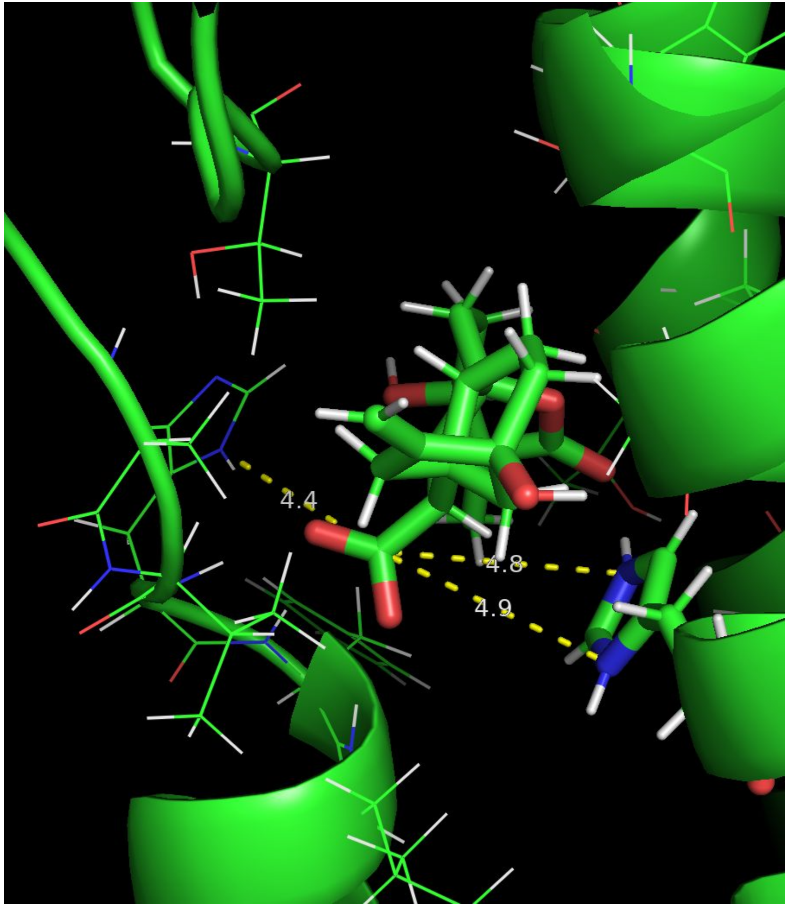
Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
33513	./3c/post_complexminimize_energy.csv-system.round_3.fin.cm.bgf	-83,0930	7	15	-436,2520	-123,7134	8	-436,2520	-384,8960	72,3574	-15,9980	-50,8790	-16,2160

S_bridge	H_bond
1	3



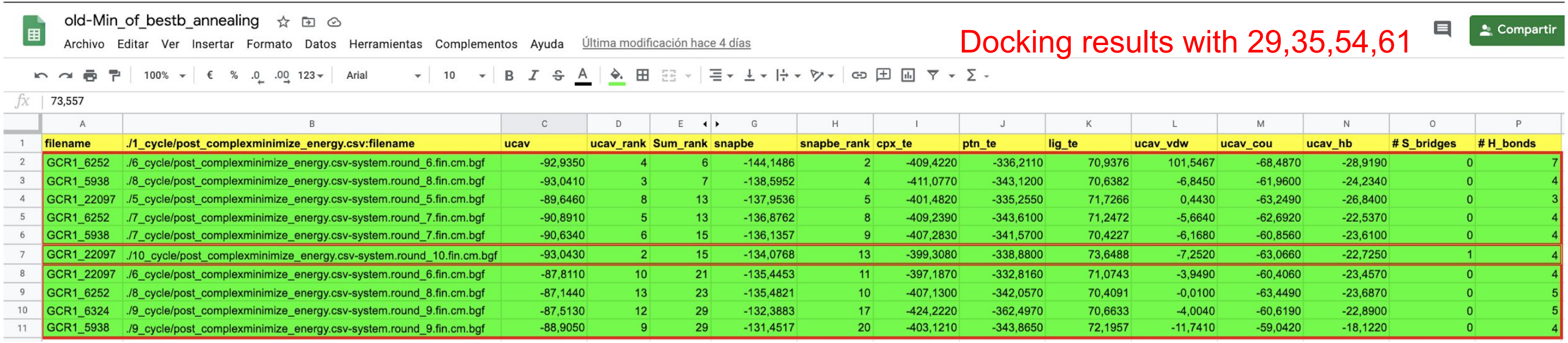


Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb
33566	./8c/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-86,5200	6	17	-402,9980	-122,5472	11	-402,9980	-354,7730	74,3222	-6,8040	-59,8780	-19,8400



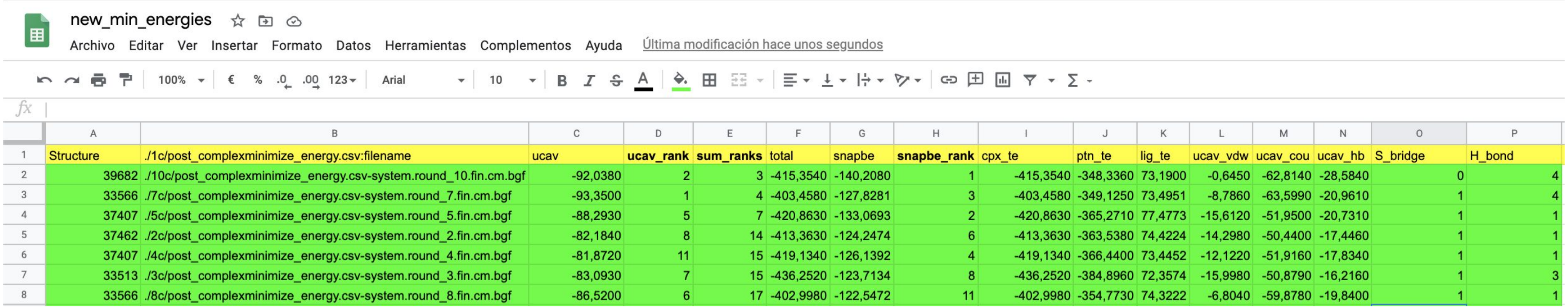
S_bridge	H_bond
1	1

Docking results with 29,35,54,61

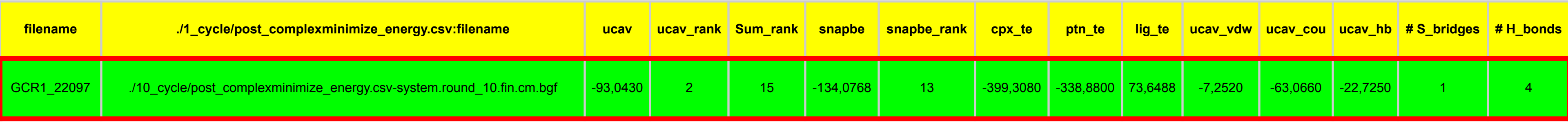


	A	B	C	D	E	G	H	I	J	K	L	M	N	O	P
1	**filename**	**./1_cycle/post_complexminimize_energy.csv:filename**	**ucav**	**ucav_rank**	**Sum_rank**	**snapbe**	**snapbe_rank**	**cpx_te**	**ptn_te**	**lig_te**	**ucav_vdw**	**ucav_cou**	**ucav_hb**	**# S_bridges**	**# H_bonds**
2	GCR1_6252	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-92,9350	4	6	-144,1486	2	-409,4220	-336,2110	70,9376	101,5467	-68,4870	-28,9190	0	7
3	GCR1_5938	./8_cycle/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-93,0410	3	7	-138,5952	4	-411,0770	-343,1200	70,6382	-6,8450	-61,9600	-24,2340	0	4
4	GCR1_22097	./5_cycle/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-89,6460	8	13	-137,9536	5	-401,4820	-335,2550	71,7266	0,4430	-63,2490	-26,8400	0	3
5	GCR1_6252	./7_cycle/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-90,8910	5	13	-136,8762	8	-409,2390	-343,6100	71,2472	-5,6640	-62,6920	-22,5370	0	4
6	GCR1_5938	./7_cycle/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-90,6340	6	15	-136,1357	9	-407,2830	-341,5700	70,4227	-6,1680	-60,8560	-23,6100	0	4
7	GCR1_22097	./10_cycle/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-93,0430	2	15	-134,0768	13	-399,3080	-338,8800	73,6488	-7,2520	-63,0660	-22,7250	1	4
8	GCR1_22097	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-87,8110	10	21	-135,4453	11	-397,1870	-332,8160	71,0743	-3,9490	-60,4060	-23,4570	0	4
9	GCR1_6252	./8_cycle/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-87,1440	13	23	-135,4821	10	-407,1300	-342,0570	70,4091	-0,0100	-63,4490	-23,6870	0	5
10	GCR1_6324	./9_cycle/post_complexminimize_energy.csv-system.round_9.fin.cm.bgf	-87,5130	12	29	-132,3883	17	-424,2220	-362,4970	70,6633	-4,0040	-60,6190	-22,8900	0	5
11	GCR1_5938	./9_cycle/post_complexminimize_energy.csv-system.round_9.fin.cm.bgf	-88,9050	9	29	-131,4517	20	-403,1210	-343,8650	72,1957	-11,7410	-59,0420	-18,1220	0	4

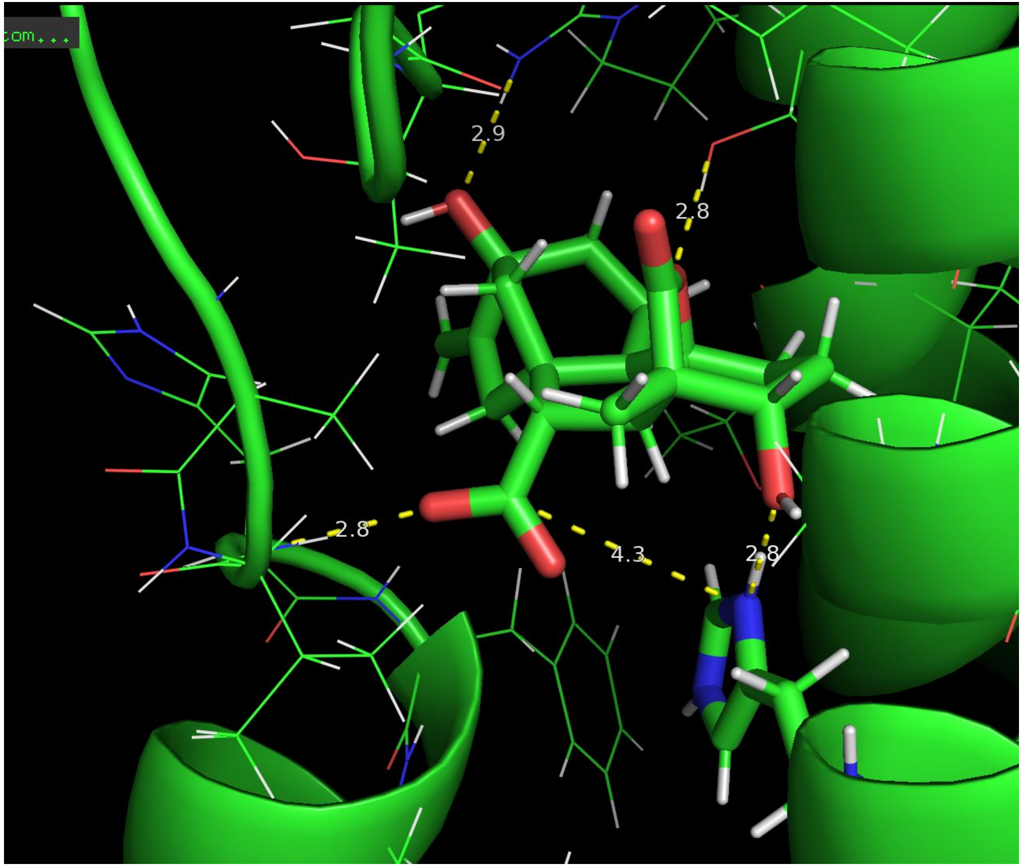
Docking results with 29,55



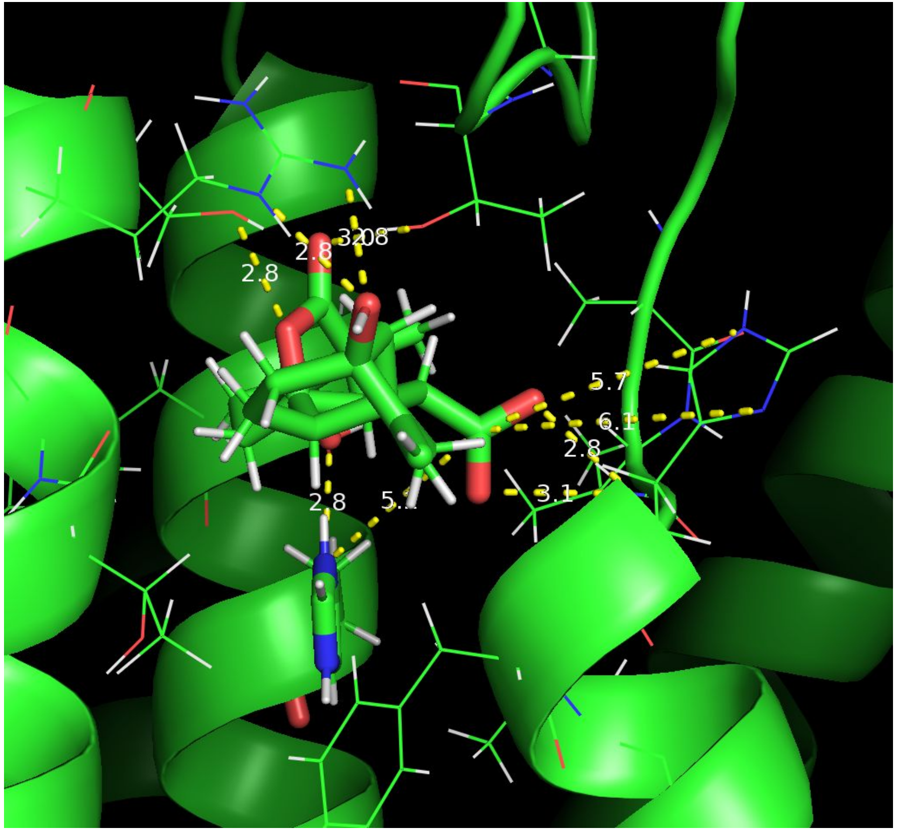
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Structure	./1c/post_complexminimize_energy.csv:filename	ucav	**ucav_rank**	**sum_ranks**	total	snapbe	**snapbe_rank**	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	S_bridge	H_bond
2	39682	./10c/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-92,0380	2	3	-415,3540	-140,2080	1	-415,3540	-348,3360	73,1900	-0,6450	-62,8140	-28,5840	0	4
3	33566	./7c/post_complexminimize_energy.csv-system.round_7.fin.cm.bgf	-93,3500	1	4	-403,4580	-127,8281	3	-403,4580	-349,1250	73,4951	-8,7860	-63,5990	-20,9610	1	4
4	37407	./5c/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-88,2930	5	7	-420,8630	-133,0693	2	-420,8630	-365,2710	77,4773	-15,6120	-51,9500	-20,7310	1	1
5	37462	./2c/post_complexminimize_energy.csv-system.round_2.fin.cm.bgf	-82,1840	8	14	-413,3630	-124,2474	6	-413,3630	-363,5380	74,4224	-14,2980	-50,4400	-17,4460	1	1
6	37407	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-81,8720	11	15	-419,1340	-126,1392	4	-419,1340	-366,4400	73,4452	-12,1220	-51,9160	-17,8340	1	1
7	33513	./3c/post_complexminimize_energy.csv-system.round_3.fin.cm.bgf	-83,0930	7	15	-436,2520	-123,7134	8	-436,2520	-384,8960	72,3574	-15,9980	-50,8790	-16,2160	1	3
8	33566	./8c/post_complexminimize_energy.csv-system.round_8.fin.cm.bgf	-86,5200	6	17	-402,9980	-122,5472	11	-402,9980	-354,7730	74,3222	-6,8040	-59,8780	-19,8400	1	1

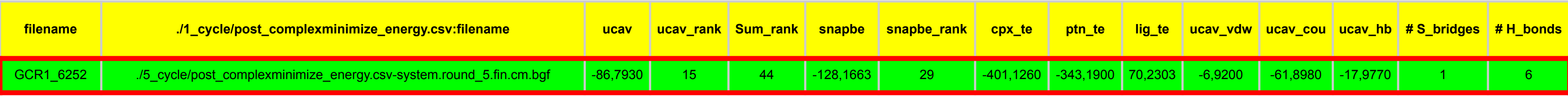


filename	./1_cycle/post_complexminimize_energy.csv:filename	ucav	ucav_rank	Sum_rank	snapbe	snapbe_rank	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	# S_bridges	# H_bonds
GCR1_22097	./10_cycle/post_complexminimize_energy.csv-system.round_10.fin.cm.bgf	-93,0430	2	15	-134,0768	13	-399,3080	-338,8800	73,6488	-7,2520	-63,0660	-22,7250	1	4

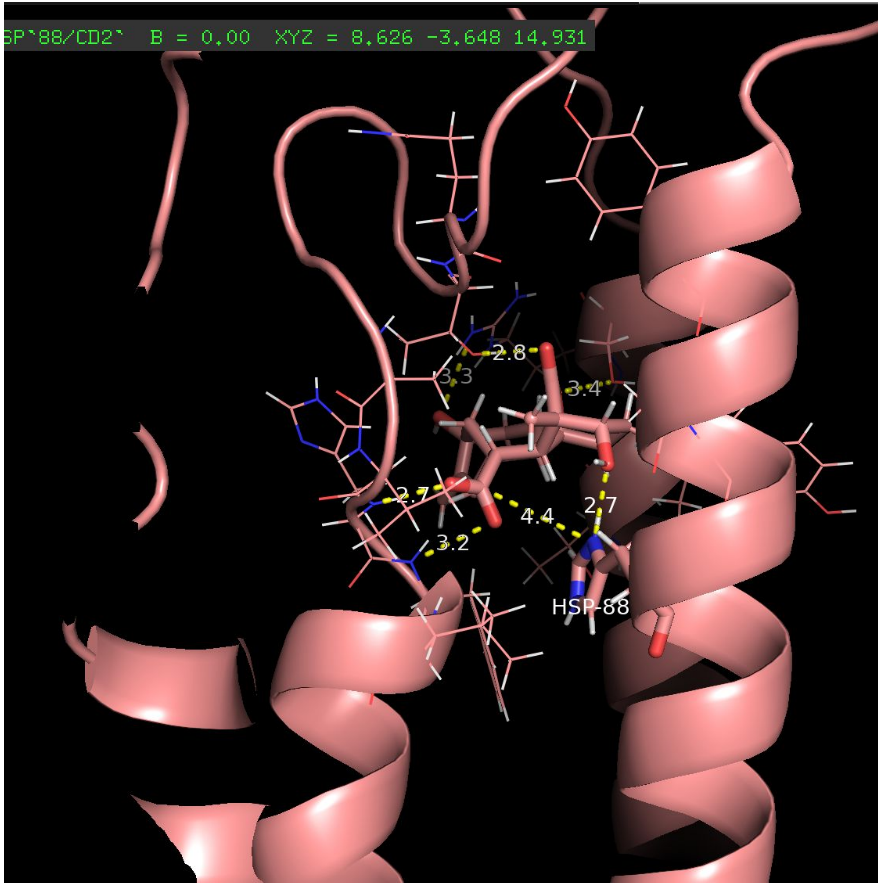


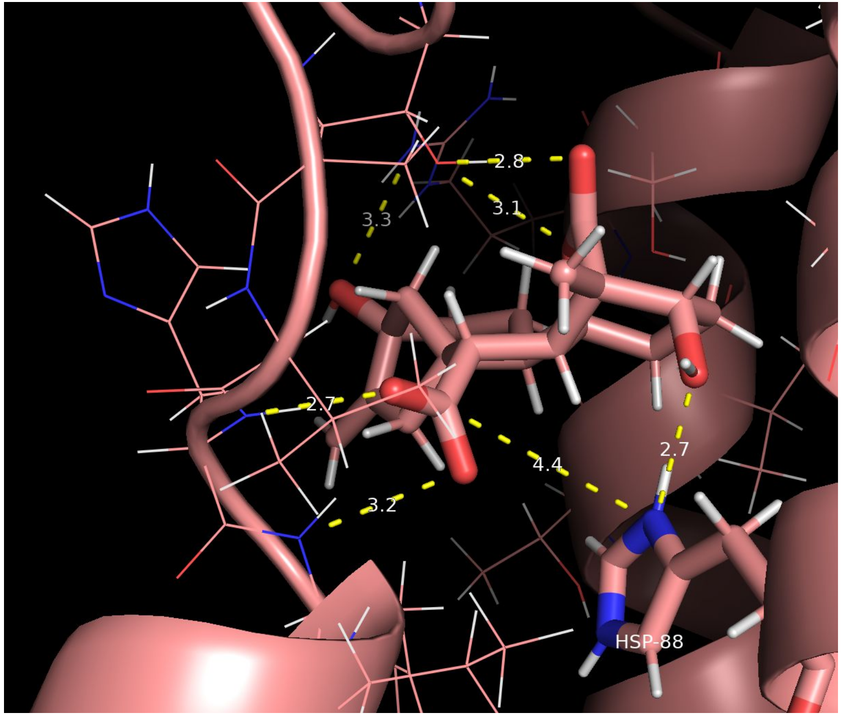
filename	./1_cycle/post_complexminimize_energy.csv:filename	ucav	ucav_rank	Sum_rank	snapbe	snapbe_rank	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	# S_bridges	# H_bonds
GCR1_6252	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-92,9350	4	6	-144,1486	2	-409,4220	-336,2110	70,9376	101,5467	-68,4870	-28,9190	0	7



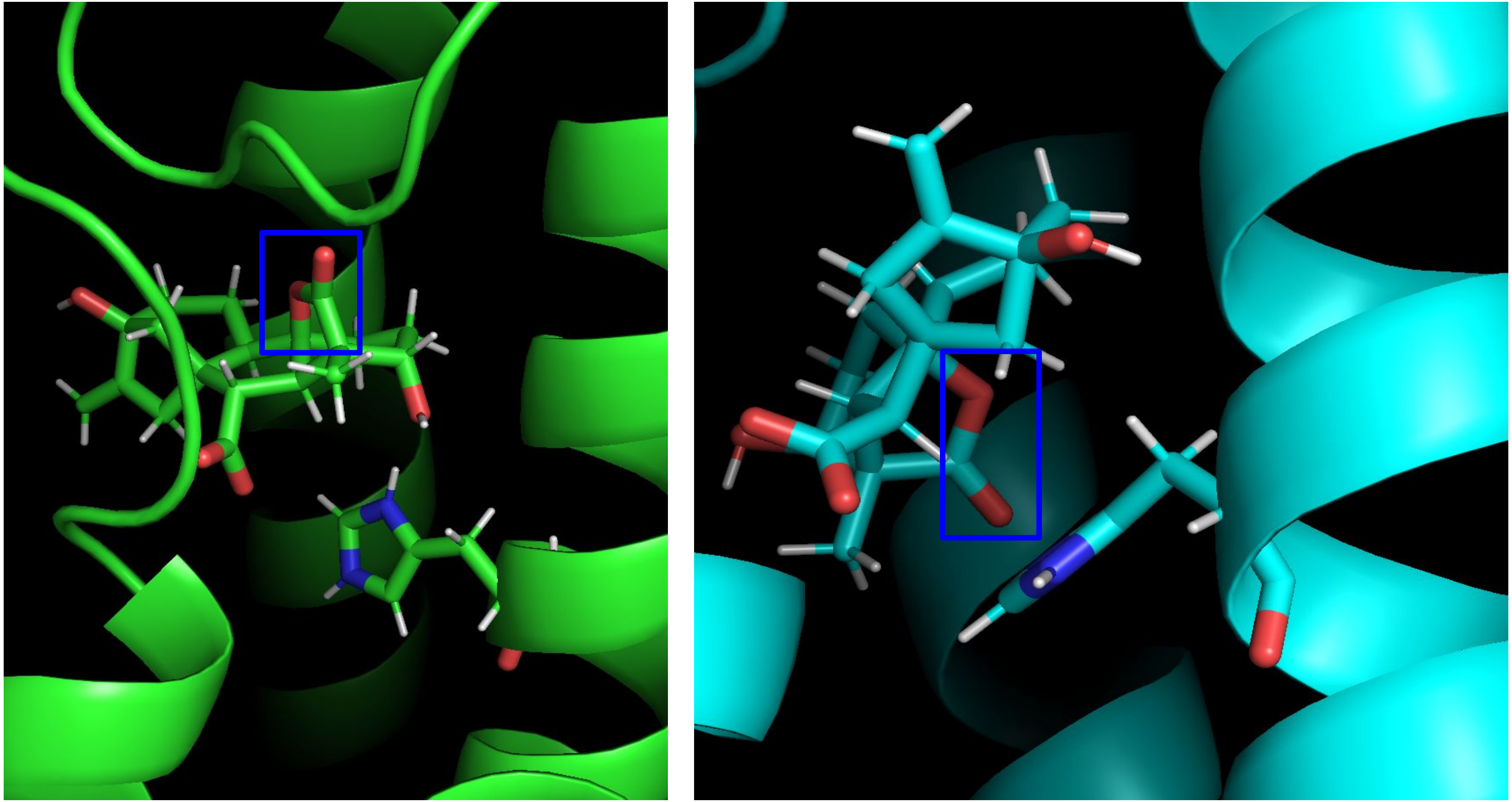


filename	./1_cycle/post_complexminimize_energy.csv:filename	ucav	ucav_rank	Sum_rank	snapbe	snapbe_rank	cpx_te	ptn_te	lig_te	ucav_vdw	ucav_cou	ucav_hb	# S_bridges	# H_bonds
GCR1_6252	./5_cycle/post_complexminimize_energy.csv-system.round_5.fin.cm.bgf	-86,7930	15	44	-128,1663	29	-401,1260	-343,1900	70,2303	-6,9200	-61,8980	-17,9770	1	6

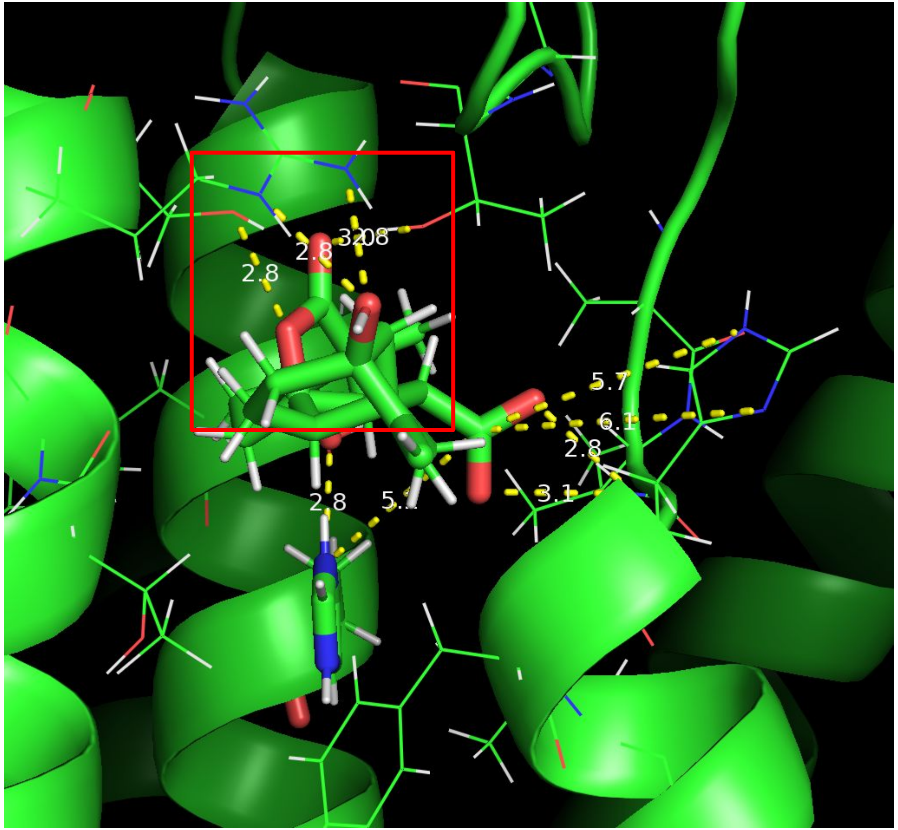


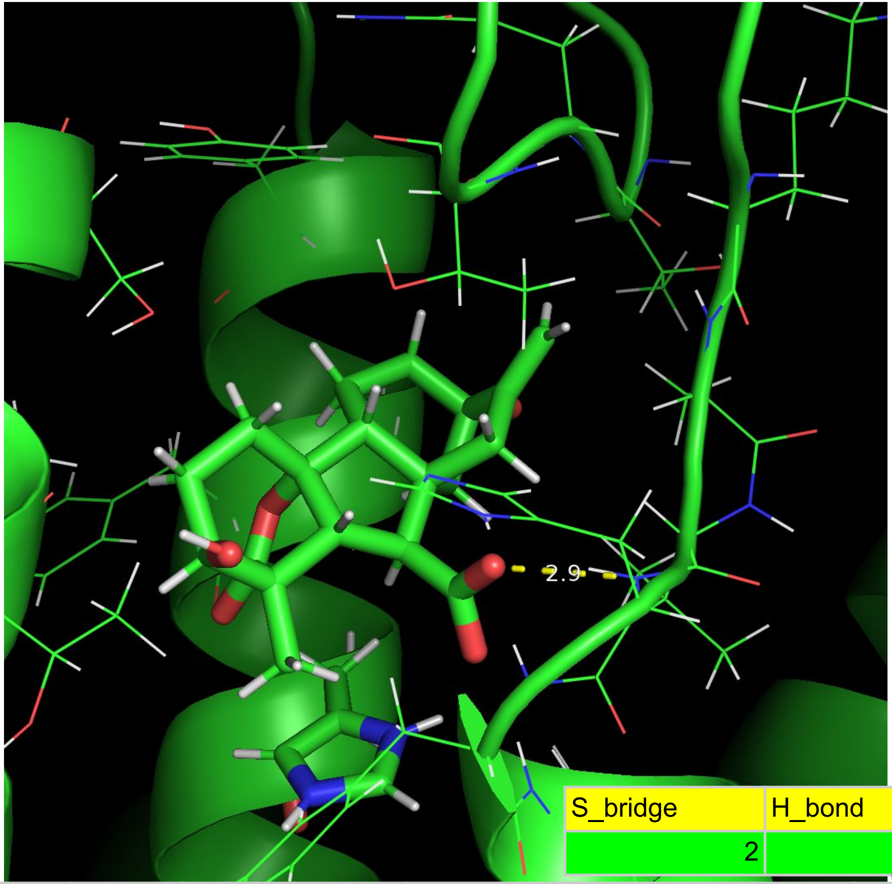


Best poses of Gibberellin A1 on 03 Ci_GCR1



GCR1_6252	./6_cycle/post_complexminimize_energy.csv-system.round_6.fin.cm.bgf	-92,9350	4	6	-144,1486	2	-409,4220	-336,2110	70,9376	101,5467	-68,4870	-28,9190	0	7





S_bridge	H_bond
2	1

37407	./4c/post_complexminimize_energy.csv-system.round_4.fin.cm.bgf	-81,8720	11	15	-419,1340	-126,1392	4	-419,1340	-366,4400	73,4452	-12,1220	-51,9160	-17,8340

Thanks

Acknowledgments

Este trabajo ha sido financiado por el Programa ÓMICAS: Optimización Multiescala In-silico de Cultivos Agrícolas Sostenibles (Infraestructura y validación en Arroz y Caña de Azúcar), patrocinado dentro del Ecosistema de Colombia Científica, conformado por el Banco Mundial, Ministerio de Ciencia Tecnología e Innovación (Minciencias), Icetex, Ministerio de Educación y Ministerio de Industria y Turismo, Proyecto ID: FP44842-217-2018.

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3. Andrés Jaramillo-Botero,Director of "Multiscale Science and Simulation Center, Caltech" and Director of OMICAS Project: In-silico Multiscale Optimization of Sustainable Agricultural Crops
4. Carlos A. Arango M. Profesor y jefe del Departamento de Ciencias Químicas. Universidad Icesi, Cali- Colombia
5. Thaura Ghneim Herrera. Profesora asociada. Laboratorio de Fisiología Vegetal. Facultad de Ciencias Naturales. Universidad Icesi
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