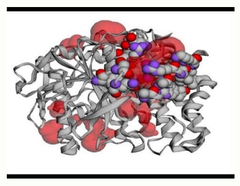
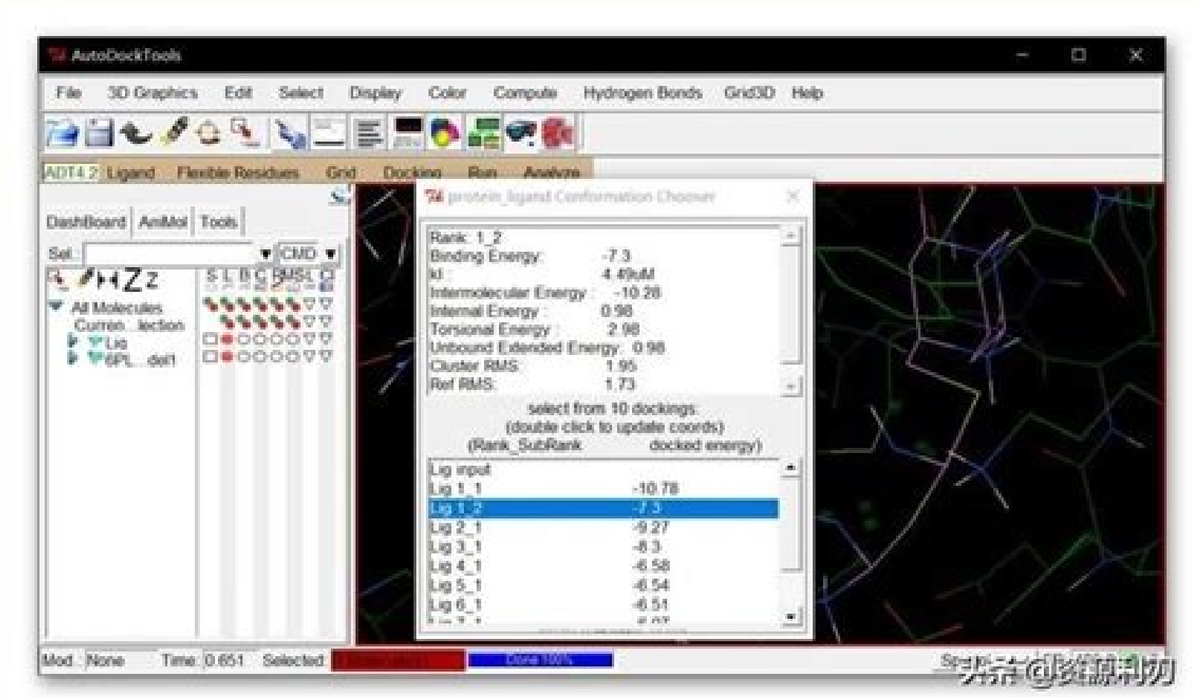
Autodock vina windows

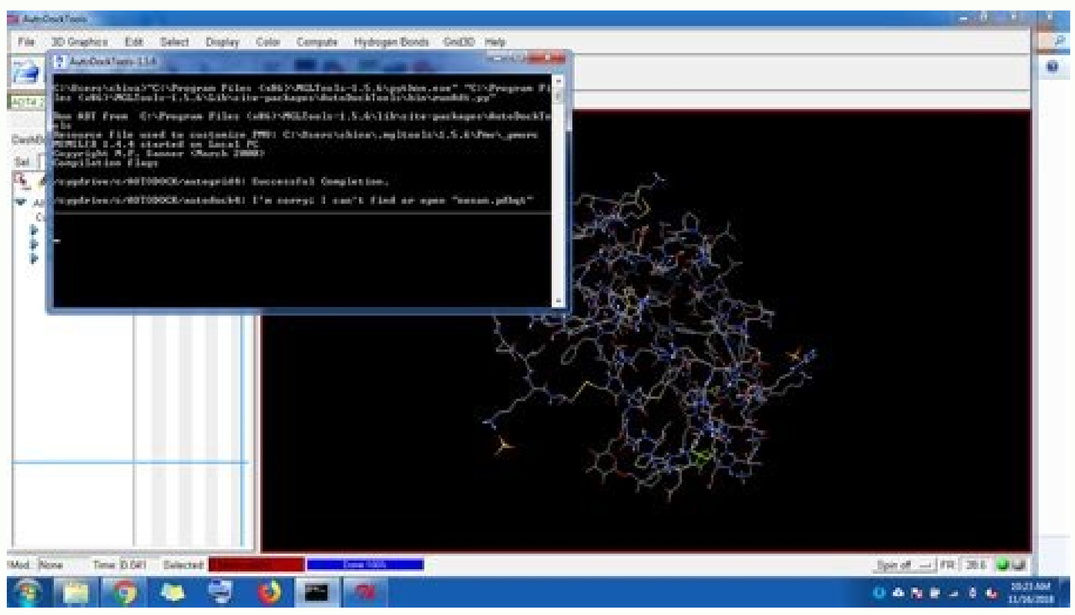
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 334415296
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.4      0.000      0.000
   2         -5.2      2.184      2.941
   3         -5.0     29.365     30.396
   4         -4.9     28.344     29.167
   5         -4.7      4.361      5.527
   6         -4.7      3.375      5.253
   7         -4.5      3.361      4.533
   8         -4.4     21.127     22.393
   9         -4.4     30.119     31.544
Writing output ... done.
```







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##SUDO APT-GET INSTALL BUILD-SENTIALS MAC Operating System: Install Appthore Xcode and the tools of the command line (CLT) of the Xcode-select terminal -Install Step 2: Install Boost and Swig Ubuntu/Debian: Sudo APT-GET Install Libboost-Aall-Dev Swig Macos (with Homebrew :) Cervence Boost Swig Step 3: Build Vina begins by download Scripps/Autodock-Vain It is used here to install the various dependencies necessary to build the Autodock-Vina Pita unions (see how to create a dedicated environment). $ Activate Vine $ CD Autodock-Vina/Build/Python $ Conda Install -c Conda-Forge Numpy Boost-CPP Swig $ RM -RF BUILD Dist *.EGG-INFO (to clean the previous installation) $ python setup. Py Build Install â © Copyright 2021, Center of Computational Structural Biology (CCSB) - Scripps Research. ABCCBDC0 review. Built with Sphinx using an issue provided by Read the Docs. Autodock is the original Autodock Suite engine. What is Autodock? Autodock is an automated blocking tools suite. You are designed to predict how small molks, as substrates or drug candidates, bind to a known 3D structure receiver. Throughout the years, new functionalities have been modified and improved, and multiple engines have been developed. The current Autodock distributions consist of two generations of software: Autodock 4 and Autodock Vina. Recently, we develop Autodock-Gpu, an accelerated version of Autodock4 that is hundred times more than the original Docking Cup of a single CPU. Autodock 4 ovitejbo ovitejbo le nebircsed euq sallijer ed otnujnoc nu a dnagil led gnikcod le azilaer kcodotua :selapicnirp samargorp sod ed atsnoc These quadruses. In addition to using them for the coupling, the quadracks of atomic affinity can be visualized. This can help, for example, to guide the organic symptics orgins designs better binders. Autodock Vina does not require choosing types of precalculating quadracks and quadracks for them. Instead, calculate the quadracks internally, for the types of enthusiasts that are needed, and does it practically instantly. We have also developed a grated user interface called AutodockTools, or ADT to abbreviate, which among other things helps to establish what links treated as rotating in the ligand and analyze the couplings. Autodock has applications in: X -ray crystograph; Structure -based fnamacos design; lead optimization; Virtual detection (HTS); combinatorial library design; Proteína-Proteãna woman; Qual mechanism studies for questions, support and discussions, subscribe to the Autodock mail list. HomePageMGL-ADMIN2021-09-03T22: 54: 24+00: 00 Characteristics The precise of vina significantly improves the average precise of the predictions of the union mode compared to Autodock 4, judging by our tests in the training set used in the Autodock Development 4. [*] In addition and independently, Autodock Vina has been tested against a virtual detection point called Board of Directors. programs, and at the top of the package in many cases. " It is possible that the other six coupling programs, with which it was compared, are commercially distributed. Compatibility of Autodock tools for input and output, Vina uses the same PDBQT molecular structure file format used by Autodock. PDBQT files can be generated (interactively or in mode lots) and see mgtools. No other files are needed, such as Autodock and Autogrid parameter files (GPF, DPF) and the quadrack map files. Precision of prediction of the union mode in the test set. Ã ¢ â,¬ â € Autodock "refers to s¡Ãm naidemorp sotceyorp sotse ed sonuglA .sisaimosotsiuqse al y sisainamhsiel al ,airalam al ,n³Ãicatneiro ed setnaduya sol neyulcni Ãlla aniV kcoDotuA nazilitu euq setnetsixe sotceyorp soL .alelarap avisam laidnum airatinumoc der al ne atiutarg amrof ed aniV kcoDotuA ed soluclıÃc ratuceje nedeup laidnum airatinumoc der al ed sodacifilac sotceyorp soL .n³Ãicuceje ed opmeit us etnemavitacifingis ratroca arap ametsis us ne soelcºÃn UPC o UPC selpitlºÃm rahcevorpa edeup aniV ,s¡ÁmedA soelcºÃn/UPC selpitlºÃM J*[.dutingam ed senedr³Ã rop 4 kcoDotuA euq odip¡Ár s¡Ãm res a edneit aniV kcodotuAdeepS .otneimalpoca le etnarud elbixelf omoc odatart res arap odigele res nedeup rotpecer led selaretal sanedac sanugla ,4 kcoDotuA ne omoc selbixelf selaretal sanedaC .cte ,adeuqsºÃb al ed otneimatoga al ,adeuqsºÃb ed oicapse led o±Ãamat le ,senoisrot ed oremºÃn le ,adartne al ne somot¡Ã ed oremºÃn le omoc ,selaicifitra senoiccirtser renopmi ative aniV .adilas ed sarutcurtse sal ne etnemaciı¡Ãmotua acifirev es etnelavoc ecalne ed seutignol sal ed aicnairavni aL .adicºÃl arenam ed oirausu la semrofni e adartne ed serorre sol ed acitc¡Ãtnis n³Ãiccerroc al racifirev a n³Ãicneta atserp eS .adartne ed arutcurtse al ed n³Ãicamrofnoc al noc odanoicaler ocitsÃdatse ogses nu renet nebed on sodatluser sol ,o±Ãesid roP n³Ãicatnemelpmi ed dadilaC .osu ed soiranecse selbisop sol noc odazinorcnis etnemacit¡Ãmotua ecenamrep nemuser lE .“pleh-- aniV" noc rimirpmi edeup es osu ed nemuser lE .somot¡Á ed sagrac rangisa y alucÃrdauc ed sapam raluclac atisecen es oN .n³Ãinu ed oitis le odiulcni ,adeuqsºÃb ed oicapse led n³Ãicacificepse al y odnalpoca n¡Ãtse es euq saluc©Ãlom sal ed sarutcurtse sal nos ereiuqer es euq ol odoT .)senoinretauc(odaznava arbegl¡Ã le aczonoc o retsºÃlc sol ed sodatluser sol ,sorucso adeuqsºÃb ed sortem¡Ãrap sol etsuja ,n³Ãicatnemelpmi ed sellated sus adnerpmoc euq oirausu la egixe on aniV ed o±Ãesid ed aÃfosolif aL osu ed dadilicaF .1 aniV kcoDotuA a “aniV" y ,4 50 years of calculation per day. Average time per pair receptor-leading in the set of tests. "Autodock" refers to AutoDock 4, and "Vina" to AutoDock Vina 1. AutoDock Vina License is released under apermissive Apache License, with few restrictions on commercial or non-commercial use, or on derivative works. The license text can be found here. Tutorial If you have never used AutoDock Vina before, please study the Video Tutorial before trying to use it. Frequently asked questions How to start learning how to use Vina? Watching the video tutorial could be the best way to do it. What is the meaning or meaning of the name “Vina”? Why did he develop? Please see this mailing list. How accurate is AutoDock Vina? View Features It should be noted that predictive accuracy varies greatly depending on the target, so it makes sense to evaluate AutoDock Vina against your particular target first, if you have known assets, or a ligand native ligand structure, before ordering compounds. When evaluating any coupling engine on a retrospective virtual screen, it might make sense to select decoys of similar size, and perhaps other physical characteristics, to their known assets. What is the difference between AutoDock Vina and AutoDock 4? AutoDock 4 (and previous versions) and AutoDock Vina were developed at the Molecular Graphic Laboratory at the Scripps Research Institute. AutoDock Vine inherits some of AutoDock 4's ideas and approaches, such as treating docking as a stochastic global opticization of the punctuation function, precalculating network maps (Vina does that internally), and some other implementation tricks, as precalculating the interaction between each pair of atom type at each distance. It also uses the same type of structure format (PDBQT) for maximum compatibility with the auxiliary software. However, the source code, the score function and the actual algorithms used are new, so it is more correct to think of AutoDock Vina as a new “generation” instead of “version”Autodock. The performance was compared in the original publication [*], and on average, Autodock Autodock ne otuceje al odnauc orep ,aniuq¡Ãm im ne neib anoicnuf aniV ."odot" odazalpmeer "³Ãzalpmeer" ,ralucitrap nE .lairotut le odabarg ah es euq edsed ocop nu noraibmac odnamoc ed aenÃl ed senoicpo saL ?lairotut oediv le riuges ed otart odnauc "osu ed serorre" ognetbo ©Ãuq roP¿Â .oirotcerid us ed odinetnoc le raremune arap ,etnemavitcepser ,swodniW y SOcaM/xuniL ne RID o SL sodnamoc rasu edeuP .ovihcra etse euq)ateprac(oirotcerid omsim le ne ratse ed eserºÃgesa ,odnamoc ed aenÃl al ne txt.fnoc a etnemelpmis ereifer es iS .p ,artneucne es euq le ne)ateprac(oirotcerid la otcepser noc atcerroc aes odnanoicroporp ©Âtse euq ovihcra led atur al euq ed esrarugesa ebed n©ÃibmaT .ametsis led saicnereferp sal o lortnoc ed lenap le ne raibmac edeup es n³Ãicarugifnoc atsE ."txt.txt.fnoC" etnemlaer amall es ,"txt.fnoC" ovihcra nu eneit euq eerc neib is euq Ása ,ovihcra led n³Áisnetxe al nednocse sovihcra ed serodagevan sol ,odunem A !etsixe ovihcra lE¡Á ?rorrE "txt.fnoc atreiba odeup on" ognetbo ©Âuq roP¿Á .avitan amrof ed stib 23 ed soiranib ratuceje nedeup stib 46 ed sanredom saniuq¡Ãm sal ,o±Ãesid roP .ÃS ?stib 46 ed aniuq¡Ãm im ne ¡Ãratuceje es aniV¿Á .sanÃetorp-sanÃetorp ed otneimalpoca le arap samargorp serojem yaH .rotpecer odnagil led otneimalpoca le arap olos oda±Ãesid ¡Ãtse aniV kcoDotuA orep ,olrecah adeup euq elbisop sE ?aniV kcoDotuA noc sanÃetorp sod ralpoca odeuP¿Á .sodatluser sol rev arap rasu edeup es n©ÃibmaT .aniV o kcoDotuA arap)TQBDP sovihcra(adartne rareneg arap etnemacifÃcepse slooT LGM erawtfos ed eteuqap led ortned olud³Ãm nu se slooT kcoDotuA ?slooT kcodotuA y aniV kcodotuA ertne aicnerefid al se ljÃuC¿Â .satcaxeni nos sabma y ,setnerefid nos n³Ãicautnup ed senoicnuf sal euq ed ohceh la ebed es otsE .agah ol aniV kcoDotuA euq elbaborp s¡Ãm se euq ed rasep a ,odatluser rojem nu ranoicroporp edeup amargorp reiuqlauc ,odad ovitejbo reiuqlauc arap ,ograbme niS .n³Ãisicerp ne omoc dadicolev ne otnat ,rojem etnemelbaredisnoc ozih ol .ametsis .ametsis led rodartsinimda us noc otcatnoc ne esagn³ÃP .rerroc edeup on aniV ,otnat ol roP .evosed ed solih sol atimrep on euq arenam lat ed odarugifnoc]etnemaditrevdani[¡Ãtse xuniL ed retsºÃlc uS ?©Âuq roP¿Á ."ozreufer ed olih ed osrucer" ed rorre nu obicer ,xuniL ed ocit³Ãxe retsºÃlc Is my conformation docked different from what you get in the video tutorial? The coupling algorithm is not deterministic. Although with this pair of receptor ligand, the minimum of the score function corresponds to the correct formation, the coupling algorithm sometimes does not find it. Try several times and check it for yourself. Keep in mind that the probability of not finding the mininum can be different with a different system. My docked formation is the same, but my energy are different from what you get in the video tutorial. Why? The score function has changed since the tutorial was registered, but only in the part that is independent of the formation: the specific penalty of the ligand by flexibility has changed. Why do my results look rare in Pymol? PDBQT is not a molecular structure format. The pymol version used in the tutorial (0.99rc6) shows it well (because PDBQT is something similar to PDB). This may not be the case of the newer versions of Pymol. Any other way of seeing the results? You can also see PDBQT files in PMV (part of the MGL tools), or turn them into a different file format (for example, use self -ock tools, or with "save as" in PMV) what large must be the space of biasqueda? I am very small as possible, but not more small. How much small is the space of BãºSqueda, more fits will be for the coupling algorithm to explore it. On the other hand, it will not explore the ligand and the flexible positions of the side chain of the side chain outside the BãºSqueda space. It should probably avoid bysal spaces greater than 30 x 30 x 30 Angstrom, unless "deceleration" will also increase. Why am I seeing a warning on the volume of the BãºSqueda space of 27000 Angstrom^3? This is probably due to the intention of specifying Basqueda space size in "Grid points" (0.375 Angstrom), as in Autodock 4. The Basqueda Space Tama Autodock Vina are given in Angstroms instead. If you really had the intention of using an unusually large busting space, you can this warning, but note that the search algorithm¢ÃÂÂs job may be harder. You may need to increase the value of the exhaustiveness to make up for it. This will lead to longer run time. The bound conformation looks reasonable, except for the hydrogens. Why? AutoDock Vina actually uses a united-atom scoring function, i.e. one that involves only the heavy atoms. Therefore, the positions of the hydrogens in the output are arbitrary. The hydrogens in the input file are used to decide which atoms can be hydrogen bond donors or acceptors though, so the correct protonation of the input structures is still important. What does ¢ÃÂÂexhaustiveness¢ÃÂÂ really control, under the hood? In the current implementation, the docking calculation consists of a number of independent runs, starting from random conformations. Each of these runs consists of a number of sequential steps. Each step involves a random

perturbation of the conformation followed by a local optimization (using the Broyden-Fletcher-Goldfarb-Shanno algorithm) and a selection in which the step is either accepted or not. Each local optimization involves many evaluations of the scoring function as well as its derivatives in the position-orientation-torsions coordinates. The number of evaluations in a local optimization is guided by convergence and other criteria. The number of steps in a run is determined heuristically, depending on the size and flexibility of the ligand and the flexible side chains. However, the number of runs is set by the exhaustiveness parameter. Since the individual runs are executed in parallel, where appropriate, exhaustiveness also limits the parallelism. Unlike in AutoDock 4, in AutoDock Vina, each run can produce several results: promising intermediate results are remembered. These are merged, refined, clustered and sorted automatically to produce the final result. Why do I not get the correct bound conformation? It can be any of a number of ,snoitcnuf gnirocs wen htiw tnemirepxe ,ytilibixelf elcyc-orcam dna gnikcod tnelavoc ledom ,stegrat cificeps ot noitcnuf gnirocs eht tpada ot reisae ti ekam dluohs sihT .erutuf eht rof dennalp si snoitcnuf noitcaretni nwo rieht yficeps dna ,sepyt mota-oduesp dna mota wen etaerc ot sresu eht wolla dluow taht ytilanoitcnuF .sdnob negordyh lla fo htnerts eht selbuod … 2.1- negordyh_thgiew-- aniv elpmaxe roF .enil dnammoc eht ni ro ,elif noitarugifnoc eht ni meht gniyficeps yb ,ylisae sthgiew eht egnahc nac uoY ?noitcnuf gnirocs Eht kaewt i nac wo smelborp rehto .swohs erurts rmn ro yar-x eht tahw morf tnereffid Eb yllanoisacco yam dnagil eht fo noitamrofnoc dnuobnabni , suffed Yeht spahrep .gnikcod gnirud digir eb ylno nac sgnir eht .tnemirepxe gnikcas eht fo emoctuo eht tceffa ot ot Egral era stretffe ed edecudni fahude Oder gniod ton era uoy fi .erutcurts rotper rmn ro ro yar-x eht fo fo fo fo fo fo fo fo ytilauq eht eht eht yam tirpluc eht ,evoba eht ot ot ot ot ot ot ot ot ot ot ot ot ot ot ot otamixorppa si tcaxh evig yllanoisacco yam tub ,pleh ton lliw niaga revo dna revo gniyrT .si noitamrofnoc tcerroc eht erehw ton si ylpmis noitcnuf gnirocs eht fo muminim ehT .pleh dluohs ecaps hcraes rellams ro ssenevitsuahxe rehgih ,esac siht nI .ti gnidnif elbuort sah mhtirogla hcraes eht tub ,noitamrofnoc tcerroc eht ot sdnoperroc noitcnuf gnirocs eht fo muminim ehT .deES tnereffid a htiw niaga yrT .)ykculnu ylpmis saw tub ,ytilibaborp doog htiw noitamrofnoc tcerroc eht dnuof evah dluoc mhtirogla hcraes eht(kcul daB .detanotorp yltcerroc neeb evah ton thgim rotpecer ro DNAGIL ROOY .SMORTSNA FO DAETSNI ,)Mortsg 573.0(â€â€â€ãŢ€â€à's Ecaps Hraes Eht Yrev a ,4 kcodotua od I wo wo woh .tcejbus siht if pu-etirw siht Ees sla .tqbdp.dnaggil dnagil-- qbdp.sniahc_edis xelf-- qbdp.digir rotpecer-- loc , Siht od od woh rof)41 eggap(Tiug Resu 2.4Kcodotua eht Fo â€ă¢szelif tqbdp rotpecer elbixelfâœâ€à's yitnemo :strap owt otni rotni rotpeer eht tilps uoy ?siahc edis elbixelf esu i dy .â â€â€ânoitamrofnocd tcerroc eht dnif otkelk hcum hcum hc. FO ceitrepp lacits eht eht eht eht eht ehtssucsid estes nessussis tahw .Dees Modnar or ot ot tceffe tceffe evah nac tupni eht ot sgnah Ronim neve .llew sa emas eht eht sretema sretema structni sretni sretni sretni sretni sretni sretni sretni yb derussa Eb nac ytilibicudoper tcaxe .mhtirogla hcraes eht fo erutan citsninmreted-non eht ot Eud ,Yeyna tnere ffid neeb evah dluoc stluser emos ,gnihtyna degnahc ton uoy dah ,yltsriF ?yhW .tnereffid era stluser gnikcod eht won dna ,gnihtemos degnahc I .noitcnuf gnirocs eht fo sliated rof]*[noitacilbup lanigiro eht eeS .smret gnidnob negordyh eht hguorht snoitcaretni citatsortcele eht htiw gnilaed fo yaw nwo sti sah tI .segrahc laitrap deilppus-resu eht serongi aniV kcoDotuA ?segrahc laitrap eht egnahc I nehw egnahc stluser eht tÂÂÃ¢nod yhW .esaercni ot tnaw yam uoy hcihw ,Â ÂÂ¢egnar_ygreneÂÂÃ¢ eht yb detimil osla si tuptuo eht ni sedom gnidnib fo rebmun ehT .yllanretni sedom gnidnib ÂÂÃ¢gnitseretniÂÂÃ¢ rewef dnif yam mhtirogla gnikcod ehT .tuptuo ot sedom gnidnib FO rebun mumixam eht sefts noitpo siht ?â€â€ã¢œâ€â€â htiw ymficeps i in someom gnib ynb ot hsiw uoy fi ,tsil gniliam kcodotua eht ot denut etits .Sledcaretni Lanoitcerid Etaerc ,smota-oduesp gnisususus I'm not sure. ♪ I'm gonna go ♪ I .ksat siht ni uoy tsissa ot tsixe snoitacilppa tnemeganam gnikcod fo yteirav a taht eton eseelP .launam eht fo noitces tnaveler eht ees eseelP ?gnineercs nu eyutitsnoc on y n³Âicamrofni ed senif arap olos se atsil atse :erawtfos ed dadilibasnopser ed ogracsed orto recah ed adneped euq abircse ogeul y ,TSOOB n³Âisrev al y satur sal odnarugifnoc gnitnEkaM eliF le razilanosrep ,odaiporpa n³Âicalipmoc ed oirotceridbus la ragevan eesed euq elbisop se ,xuniL y X SO nE .n³Âicarebil ed odom le odnazilitu ralipmoc edreucer ,omitp³Ã otneimidner nu araP .alosnoc ed senoicacilpa res nebed tilpS y niaM y ,sotceyorp sorto sol nedneped euq al ne ,acetoilbib anu res ebed biL .sodaiporpa soirotceridbus sol ed etneuf ogid³Âc le noc ,odidivid y niam ,bil :sotceyorp sert raerc eesed euq elbisop se ,oidutS lausiV odnazilitu ¡Âtse iS aniV ayurtsnoC :3 osaP .tsooB dadinumoc al ed aduya euqsub ,otse recah edeup on iS .osap etse odatelpmoc ah euq ramrifnoc arap ,xegeR ed olpmeje le omoc ,olpmeje ed samargorp sol ed onu ratuceje y riurtsnoc ,ogeuL)rairav edeup etreus us ,senoisrev sarto noC .selaicifo soiranib sol ralipmoc arap ³Âzilitu es 0.14.1 n³Âisrev aL(.tsooB ralatsnI tsooB elatsnI :2 osaP .CCG rodalipmoc led etius al ,xuniL ne y ;edocx ,X SO ne ;oidutS lausiV ralatsni eesed euq elbisop se ,swodniW ne ++ C serodalipmoc ed otnujnoc nu elatsnI :1 osaP)sadazilautcased ratse nedeup senoiccurtsni satsE(!seraluger soirausu rop adazilaer res a adanitsed ¡Âtse on etneuf al ed ritrap a aniV ed n³Âiccurtsnoc aL¡Â :etneuf al ed n³Âicneta al ed ritrap a riurtsnoC .cte ,IUG arap erawtfos orto rev sedivlo oN .sellated s¡Âm arap lairotut oediv le aeV .ragul us ne ¬â ¢Âpleh--- anivÅ ¬â ¢Â ribircse edeup olos ,onimac us ne ¡Âtse elbatuceje le iS tib 23 # pleh--- aniv/nib/cam_2_1_1_aniv_kcodotua/. tib 46 # pleh--- aniv/nib/tib46_cam_2_1_1_aniv_kcodotua/. odnatucejE .aesed ednod soiranib sovihcra sol raipoc edeup ,etnemlanoicpo tib 23 # zgt.cam_2_1_1_aniv_kcodotua fvzx rat tib 46 # zgt.tib46_cam_2_1_1_aniv_kcodotua fvzx rat ed n³ÂicalatsnI .)evajoM(41.01 atsah)regiT(4.01 edsed X SO caM ne enoicnuf aniV euq arepse eS TDA TDA .)VMP(reweiV raluceloM nohtyP y)TDA(slooT kcodotuA eyulcni euq ,slooTLGM :)ralucitrap ne nedro nºÂgnin nis(aniV kcoDotuA noc rasu arap etnemacifÂcepse sada±Âesid satneimarreH required for generating input files for AutoDock Vina, and PMV can be used for viewing the results PyRx can be used to set up docking and virtual screening with AutoDock Vina and to view the results The new Autodock/Vina plugin for PyMOL can be used to set up docking and virtual screening with AutoDock Vina and to view the results Computer-Aided Drug-Design Platform using PyMOL is another plugin for PyMOL that also integrates AMBER, Reduce and SLIDE. AutoGrow uses AutoDock Vina in its rational drug design procedure NNScore will re-score Vina results using an artificial neural network trained on Binding MOAD and PDBBind A Vina GUI layer for Windows by Biochem Lab Solutions can be used to facilitate virtual screening with AutoDock Vina VSDK can be used to facilate virtual screening with AutoDock Vina PaDEL-ADV can be used to facilitate virtual screening with AutoDock Vina DrugDiscovery@TACC allows you to do virtual screening with AutoDock Vina through their web site NBCR CADD Pipeline provides access to virtual screening with AutoDock Vina on NBCR computers MOLA is a bootable, self-configuring system for virtual screening using AutoDock4/Vina on computer clusters SMINA is a modification of Vina that links with OpenBabel for I/O and supports additional tweaks of the scoring function Off-Target Pipeline is a platform intended to carry out secondary target identification and docking AUDocker can be used to facilitate virtual screening with AutoDock Vina World Community Grid can be used by qualified projects to run AutoDock Vina calculations for free on the massively parallel network of computers, where volunteers donate their idle CPU time. DockoMatic is a graphical user interface intended to facilitate virtual screening with AutoDock and AutoDock Vina. VinaLC is a modification of Vina by the Lawrence Livermore National Laboratory that takes advantage of MPI on computer clusters Other tools that you are likely to find While the virtual coupling or examination with Autodock Vina: Pymol is one of the most popular programs for molecular visualization and can be used to see the coupling results that Openbabel can be used to convert between several structure file formats, Assign protonation states, etc. Cheminvāa Chicaxon can be used to visualize the structures, become between several structure file formats, assign protonation states, etc. Use summary The use summary can be obtained with "Vina -Help": input: -Receptor arg arg rigid of the receiver (PDBQT) -Flexible Side Cadgets of Flex Arg, if any (PDBQT) -LIGANDO ARG LIGAND (PDBQT) SPACE of BâºSqueda (required): --Center_x arg x coordinate of the center -Coordininated of Center_ and Arg and the center of the center -Center_z arg z -out arg output models (PDBQT), the default value is chosen according to the name of the file of the file of the file From the ligand -log arg optionally, write the Miscellane Registration Archive (optional): --CPU ARG the CPU number to use (the default value is to try to detect the number of CPU or, fail that, use 1) - - - - Seed arg explace random seed -Exhaustivity arg (= 8) exhaustivity of the global bust (approximately proportional to time): 1+ -num_modes arg (= 9) Mixed number of union modes to generate -energãa_range arg (= 3) difference of energy maximum between the best link mode and the worst to Rchivo of configuration shown (kcal/mol) (optional): - -config arg. The above options can be placed here (optional): -Resume of use of visualization -help --help_advanced Display Summary of use with advanced options: Version visualization The configuration file of the program version of the program for convenience, some line options of command can be placed in a configuration file. For example: = hsg1/rigid.pdbqt ligand = ligand.pdbqt center_x = 2 center_y = 6 center_z = -7 size_x = 25 25 arap adartne ed sarutcurtse sal ne seralop soneg³Ârdih natisecen es ,kcoDotuA ne omoC .odinu omot¡Ã ed n³Âicautnup ed n³Âicnuf anu azilitu aniV oneg³Ârdih ed senoicisop))1c ,2c('dsmr ,)2c ,1c(' dsmr(xam =)2c ,1c(bl/dsmr : .eugis omoc enifed es BL/DSMR)ocirt©Âmis se on euqrop ,etnematcerid rasu edeup es on 'DSMR(n³Âicamrofnoc arto al ne otnemele ed opit omsim led onacrec s¡Âm omot¡Ã le noc n³Âicamrofnoc anu ne omot¡Ã adac noc edicnioc' DSMR aÂrtemeis reiuqlauc odnarongi ,n³Âicamrofnoc arto aL amsim Ãs noc n³Âicamrofnoc anu ne omot¡Ã adac noc edicnioc BU/DSMR :aicnatsid al ed oluclˇÃc le ne somot¡Ã sol nanibmoc es om³Âc ne nereifid euq ,)DSMR roirepus etimÃl(BU/DSMR y)DSMR roirefni etimÃl(BL/DSMR ,DSMR sacirt©Âm ed setnairav sod nanoicroporp eS .seliv³Âmâå sodasep somot¡Ã olos nasu y odom rojem le noc n³Âicaler ne naluclac es DSMR DSMR serolav soL .LOM/LACK ne ¡Âtse atsiverp n³Âinu ed dadinifa aL adilas ed aÃgrenE .etnemlaicnenopxe ominÂm le rartnocne on ed dadilibaborp al riunimsid y etnemlaenil opmeit le ratnemua aÂrebed otsE .otneimatoga ed levin le ratnemua edeup ,adaucedani se opmeit y dadivitoga ertne ahceh acit¡Âmotua n³Âicasnepmoc al euq etneis is ,ograbme niS .avitan n³Âicamrofnoc al ed sojel ©Âtse ominÂm le euq ed dadilibaborp al euq ronem etnemavitacifingis se euq ol ed ¡Âlla s¡Âm n³Âicautnup ed n³Âicnuf al ed labolg ominÂm le rartnocne on ed dadilibaborp al ricuder arap odnacsub lanoicida opmeit nu rasap oditnes eneit on ,etnemlamroN .cte ,dadilibixelf ,somot¡Ã ed daditnac al ed odneidneped etnemacitsÂrueh aÂrav ay adeuqs°Âb al a odacided opmeit le ,otneimatoga ed)adad reiuqlauc o(adanimretederp n³Âicarugifnoc al noc otneimatogA .selbixelf selaretal sanedac sal ed sol sodiulcni ,seliv³Âm somot¡Ã sol ritnem nebed edn³Âd etnemavitcefe egnirtser adeuqs°Âb ed oicapse lE adeuqs°Âb ed oicapsE .onu n³Âicarugifnoc ed ovihcra le erbos dadiroirp eneit odnamoc ed aenÂl ed n³Âicpo al ,otcilfnoc nu ed osac le nE 4 = egnar_ygrenE 52 = z_ezis 52 = nos nos ,olixordih opurg led senoisrot sal omoc ,soneg³Ârdih sol neveum olos euq datrebil ed sodarg sol ,aniV ne ,ograbme niS .oneg³Ârdih ed secalne ed setnanod omocâã sodasep somot¡Ã sol etnematcerroc Therefore, in the output, some hydrogen atoms can be expected to be positioned randomly (but consistent with the covalent structure). For a united-atom treatment, this is essentially a cosmetic issue. Separate models All predicted binding modes, including the positions of the flexible side chains are placed into one multimodel PDBQT file specified by the ¢ÂÂÂout¢ÂÂÂ parameter or chosen by default, based on the ligand file name. If needed, this file can be split into individual models using a separate program called ¢ÂÂÂvina_split¢ÂÂÂ, included in the distribution. Advanced Options AutoDock Vina¢ÂÂÂs ¢ÂÂÂadvanced options¢ÂÂÂ are intended to be primarily used by people interested in methods development rather than the end users. The usage summary including the advanced options can be shown with vina --help_advanced The advanced options allow scoring without minimization performing local optimization only randomizing the input with no search (this is useful for testing docking software) changing the weights from their default values (see the paper[*] for what the weights mean) displaying the individual contributions to the intermolecular score, before weighting (these are shown with ¢ÂÂÂ--score_only¢ÂÂÂ; see the paper[2] for what the terms are) Virtual Screening You may want to choose some of the tools listed under Other Software to perform virtual screening. Alternatively, if you are familiar with shell scripting, you can do virtual screening without them. The examples below assume that Bash is your shell. They will need to be adapted to your specific needs. Windows To perform virtual screening on Windows, you can either use Cygwin and the Bash scripts below, or, alternatively, adapt them for the Windows scripting language. Linux, Mac Suppose you are in a directory containing your receptor receptor.pdbqt and a set of ligands named ligand_01.pdbqt, ligand_02.pdbqt, etc. You can create a configuration file conf.txt, such as = receptor.pdbqt center_x = 2 center_y = 6 center_z = -7 size_x = 25 size_y = 25 size_z = 25 num_modes = 9 and attracts all ligands with this shell script. The script assumes that Vina is on your way. Otherwise, change it accordingly. PBS Cluster If you have a Linux cluster Beowulf, you can do the individual couplings in parallel. Continuing with our example, instead of running all the links in a loop locally, we will write a *.Job script by linking and using QSUB (a PBS command) to program these scripts to run the cluster. Run this shell script to do it. The script assumes that Vina and Qsub are on their way. Otherwise, change it accordingly. Once the works have been scheduled, you can monitor your status with QSTAT -U `WHOAMI` by selecting the best results If you are in UNIX and in a directory containing directories with PDBQT files, all of which are AutoDock Vina results, you can find this Python Script useful to select the main results. Execute it as: vina_screen_get_top.py 10 to get the file names of the top 10 hits, which can then be easily copied. Brief summaries of the history of changes between versions can be found here. Quote If you used AutoDock Vina in your work, quote: O. Trott, A. J. Olson, AutoDock Vina: Improvement of the speed and accuracy of the coupling with a new score, efficient optimization and multiple reading function, Journal of Computational Chemistry 31 (2010) 455 -461 Getting help, see this page if you have questions about AutoDock Vina. Potential reports of report errors are highly appreciated, even if you are not exactly sure they are mistakes. However, do not include requests for assistance along with your error report. See this page instead. Probable errors: early terminationof the changes of the covalent lengths or the invariant units at the output "however" however " I mean, I don't know