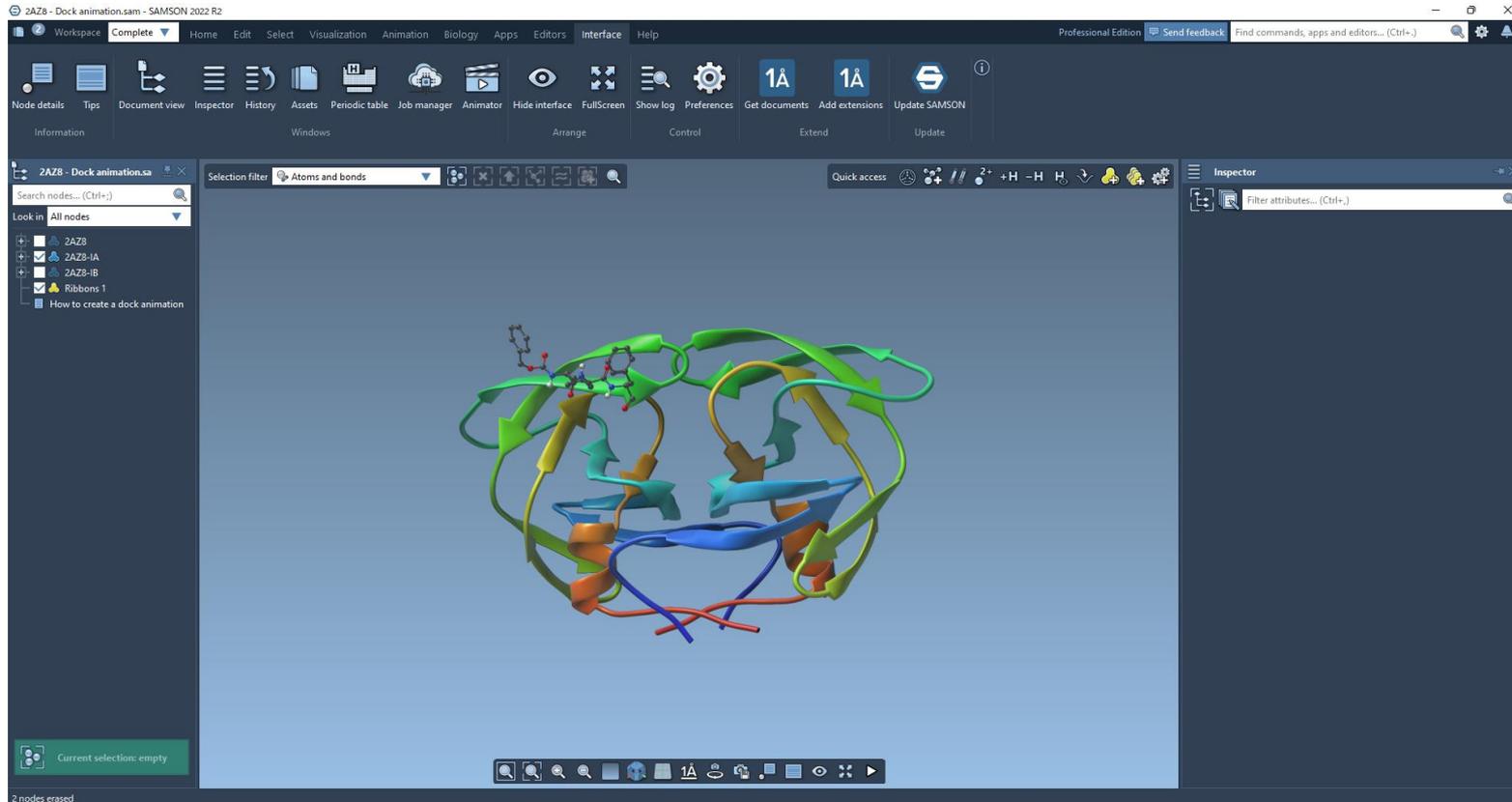


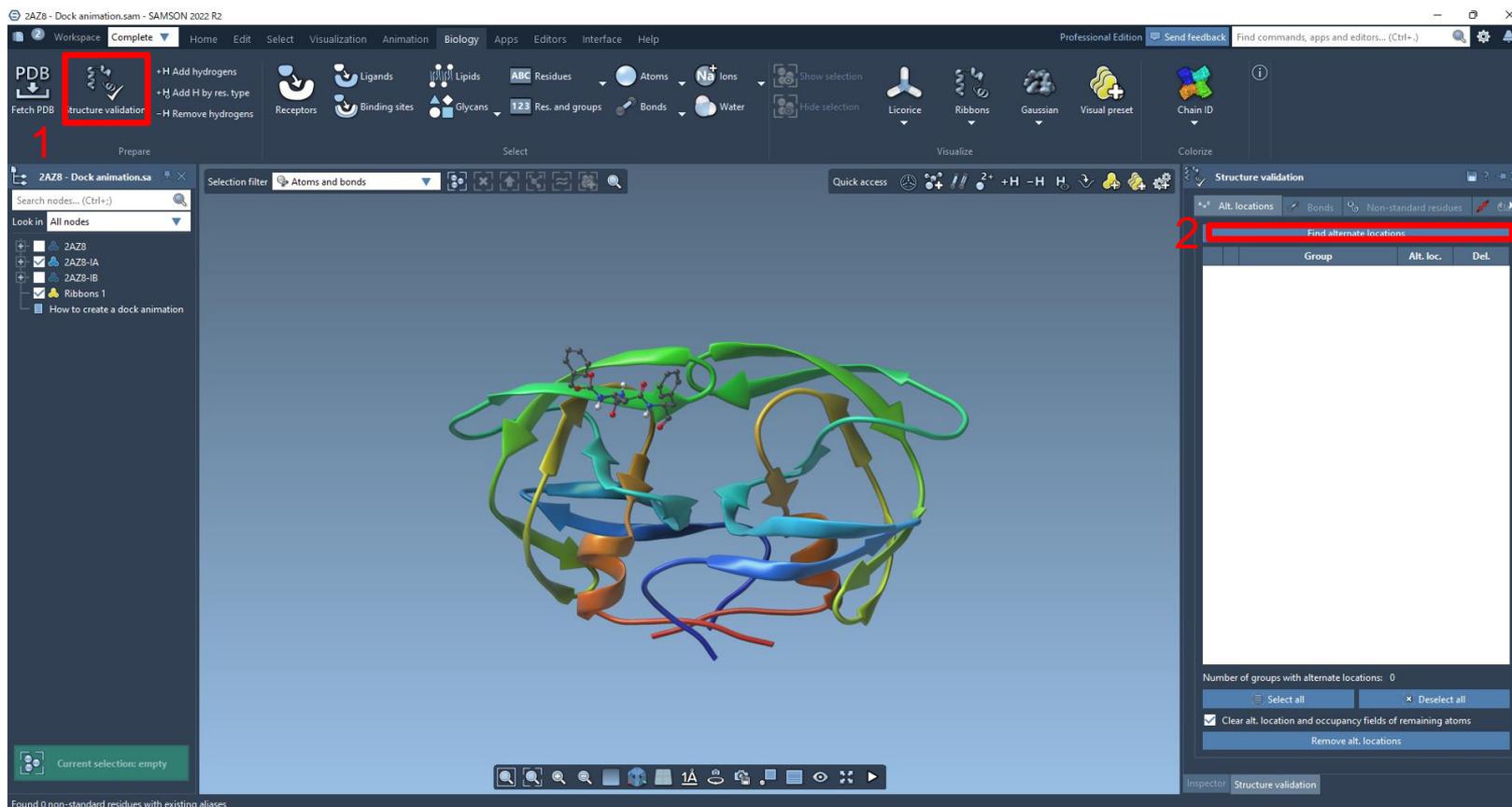
AutoDock Vina Extended によるリガンドドッキング

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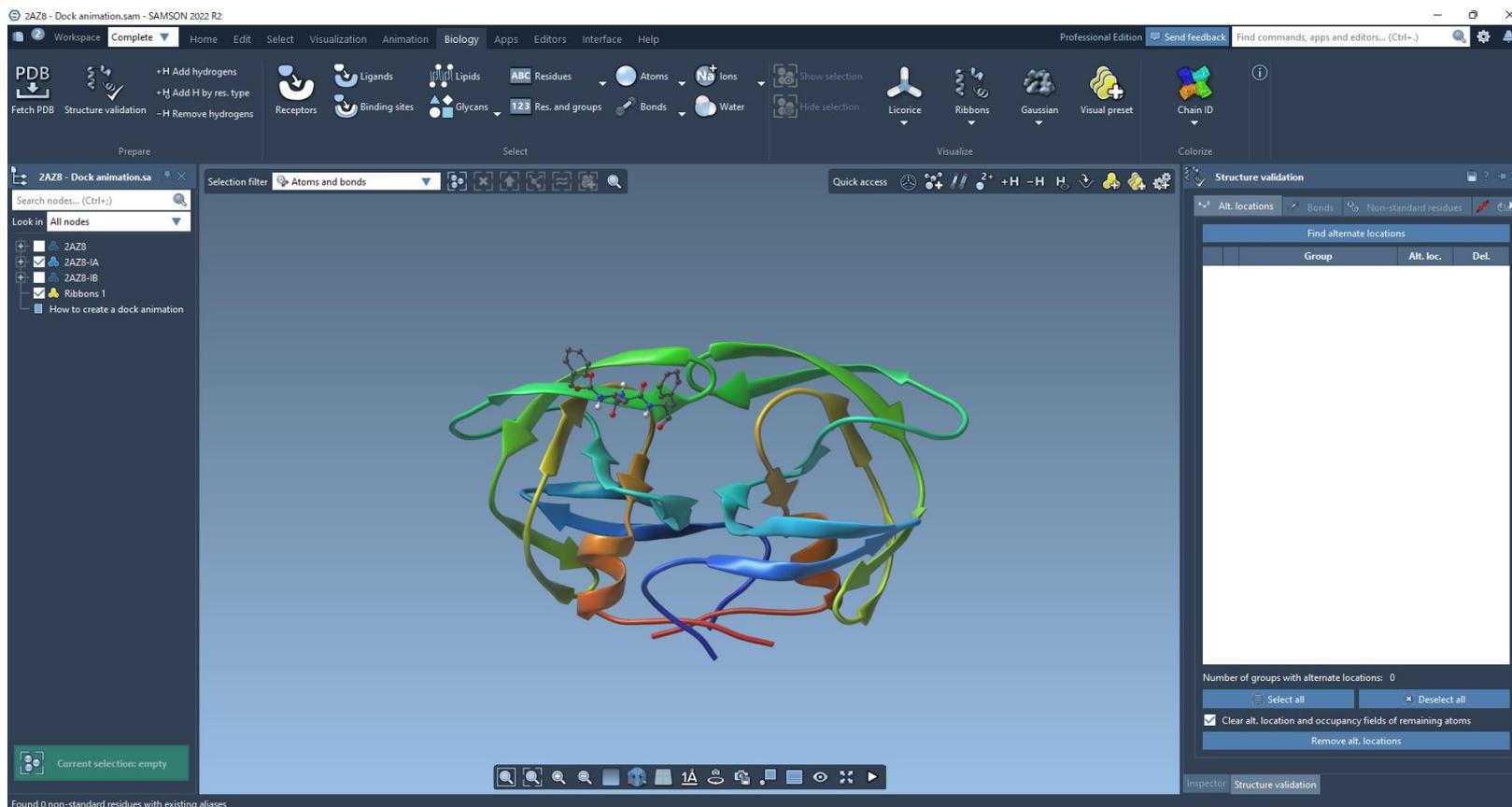
受容体・リガンドの表示



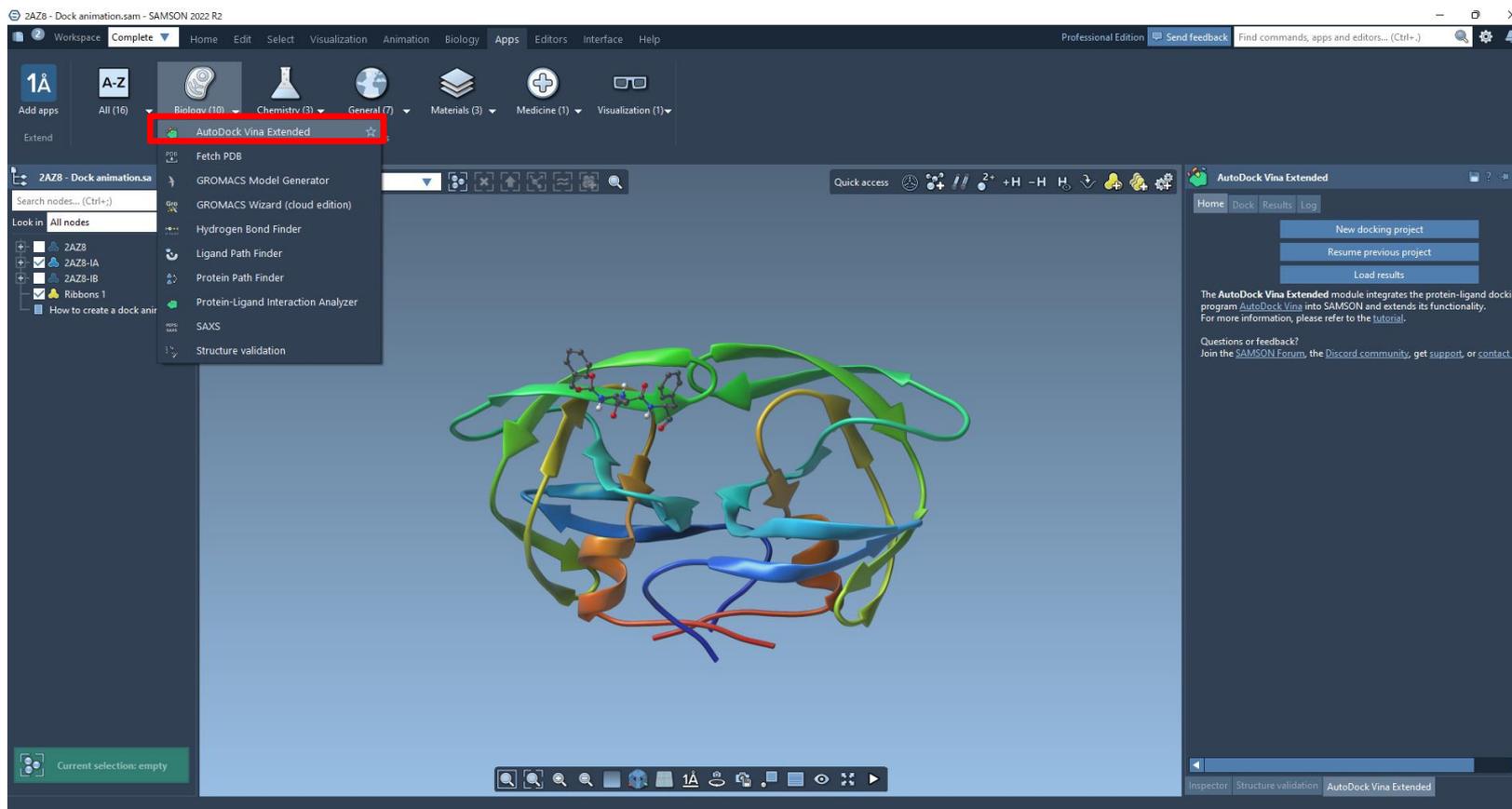
ドッキングを行う受容体とリガンドの構造を表示した状態にします。
(受容体：HIV-1タンパク質分解酵素、リガンド：TL-3)



1. Biologyメニュー中の“Structure validation”をクリックし、Alt. locations タブを表示させます。
2. “Find alternate locations”をクリックし、シミュレーションを行う上で構造データに問題がないかを検証します。



同じくBiologyメニューから必要に応じて、水分子の除去、イオンの除去、水素原子の付加も可能です。



AppメニューのAutoDock Vina Extendedをクリックし、AutoDock Vina Extendedタブを表示させます。

The screenshot displays the SAMSON 2022 R2 software interface. On the left, a sidebar shows a list of nodes under 'Look in: All nodes'. The node '2AZ8' is highlighted with a red box and a red number '1'. The main 3D view shows a protein structure with a ligand docked. On the right, the 'AutoDock Vina Extended' panel is open. The '1 - Set receptor' section has the 'Set' button highlighted with a red box and a red number '2'. Below this, the '2 - Set ligand' section is visible. The '3 - Setup search domain' section shows a table of coordinates:

Based on receptor		Set		Show box	
Center: X	0.0 Å	Y	0.0 Å	Z	23.7 Å
Size: X	57.2 Å	Y	31.9 Å	Z	40.0 Å

The '4 - Dock' section shows 'Exhaustiveness: 8' and 'Modes: 10'. The 'Save results' section shows the path 'C:/Users/IKENAGA-PC/Downloads' and a 'Save receptor in files with resulting ligand modes' checkbox. At the bottom, there are buttons for 'Dock ligand', 'Pause', and 'Stop', with a progress indicator at 0%.

1. 受容体を選択します。（受容体ライブラリー指定することも可能です。）
2. AutoDock VinaタブのReceptorでSetをクリックします。

2AZB - Dock animation.sam - SAMSON 2022 R2

Workspace Complete Home Edit Select Visualization Animation Biology Apps Editors Interface Help Professional Edition Send feedback Find commands, apps and editors... (Ctrl-)

1Å Add apps All (16) Biology (10) Chemistry (3) General (7) Materials (3) Medicine (1) Visualization (1)

Extend All apps

2AZB - Dock animation.sa

Selection filter Atoms and bonds

Quick access 2+ +H -H H

AutoDock Vina Extended

Home Dock Results Log

1 - Set receptor

Single receptor from document

Receptor Set Select

Flexible side chains 2 Set Select

Rotatable bonds Lock Unlock

2 - Set ligand

Single ligand from document

Ligand Set Select

Rotatable bonds Lock Unlock

Minimize 5000 steps Add missing hydrogens

Lock specific bonds Locked bonds settings

3 - Setup search domain

Based on receptor Set Show box

Center: X 0.0 Å Y 0.0 Å Z 23.7 Å

Size: X 57.2 Å Y 31.9 Å Z 40.0 Å

4 - Dock

Dock Exhaustiveness 8 Modes 10

Save results

C:/Users/WENAGA-PC/Downloads Open

Save receptor in files with resulting ligand modes

Dock ligand Pause Stop

0%

Inspector Structure validation AutoDock Vina Extended

Look in All nodes

ASP 30

THR 31

VAL 32

LEU 33

GLU 34

GLU 35

MET 36

ASN 37

LEU 38

PRO 39

GLY 40

ARG 41

TRP 42

LYS 43

PRO 44

LYS 45

MET 46

ILE 47

GLY 48

GLY 49

ILE 50

GLY 51

GLY 52

PHE 53

ILE 54

LYS 55

VAL 56

ARG 57

GLN 58

Current selection: 7 nodes

C29, H10, N8, O7, S1

7 residues (out of 202)

35 atoms (out of 1906)

614,514 Da (out of 21010 Da)

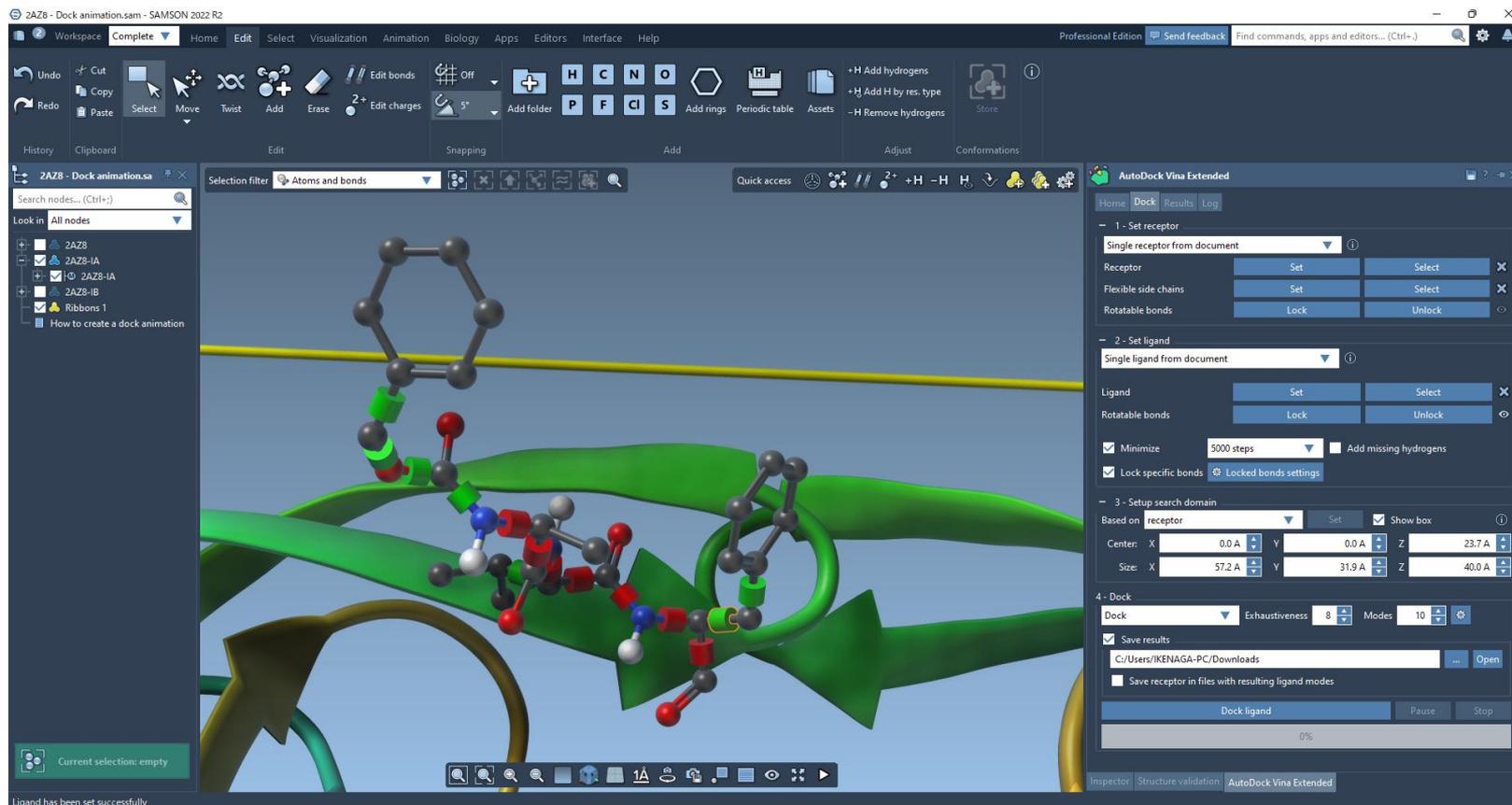
Receptor has been set

1. Flexible chainに指定する側鎖を選択します。
2. AutoDock Vina ExtendedタブのFlexible side chainでSetをクリックします。

The screenshot displays the SAMSON 2022 R2 software interface. The central 3D view shows a protein structure with a yellow bounding box. On the left, the 'Look in' panel shows a tree view with '2AZ8-IA' selected, highlighted by a red box and a red number '1'. On the right, the 'AutoDock Vina Extended' panel is open, showing the '2 - Set ligand' section where the 'Set' button is highlighted with a red box and a red number '2'. The '3 - Setup search domain' section shows a bounding box with dimensions: Center (X: 0.0 A, Y: 0.0 A, Z: 23.7 A) and Size (X: 57.2 A, Y: 31.9 A, Z: 40.0 A). The '4 - Dock' section shows 'Exhaustiveness: 8' and 'Modes: 10'. The 'Save results' section shows the path 'C:/Users/IKENAGA-PC/Downloads'.

1. リガンドを選択します。(リガンドライブラリー指定することも可能です。)
2. AutoDock Vina ExtendedタブのLigandでSetをクリックします。

結合の回転・無回転を指定



リガンドの各結合をクリックすることで、回転可能（緑）または回転不可能（赤）のいずれかを指定します。

（二重結合等、結合の特性に応じて一括で指定することも可能です。）

The screenshot displays the SAMSON 2022 R2 interface. The main window shows a protein structure with a yellow wireframe box representing the search domain. A red arrow points to the top-right corner of this box. On the right, the 'AutoDock Vina Extended' panel is open, with the '3 - Setup search domain' section highlighted in red. This section contains the following parameters:

Parameter	Value
Based on	pocket / selection
Center X	6.2 Å
Center Y	6.0 Å
Center Z	35.2 Å
Size X	32.6 Å
Size Y	17.2 Å
Size Z	24.9 Å

Below the search domain settings, the '4 - Dock' section shows 'Exhaustiveness' set to 8 and 'Modes' set to 10. The 'Save results' checkbox is checked, and the output path is 'C:/Users/IKENAGA-PC/Downloads'.

探索を行う領域を指定します。

AutoDock Vina ExtendedタブのSetup search domainまたは、黄色のボックスの頂点をドラッグすることで、サイズの変更が可能です。

The screenshot displays the SAMSON 2022 R2 software interface. The main window shows a protein structure (2AZ8) with a yellow bounding box around a specific region. A ligand is docked within this region. The left sidebar lists amino acid residues, and the bottom status bar indicates 'Current selection: CA'. The right-hand panel, titled 'AutoDock Vina Extended', contains settings for docking. The 'Dock' section is active, and the 'Dock ligand' button is highlighted with a red rectangle. Other settings include 'Exhaustiveness: 8', 'Modes: 10', and 'Save results' checked.

Dock ligandをクリックし、ドッキングを行います。

2AZ8 - Dock animation.sam - SAMSON 2022 R2

Workspace Complete Home Edit Select Visualization Animation Biology Apps Editors Interface Help

Professional Edition Send feedback Find commands, apps and editors... (Ctrl+)

Undo Cut Copy Paste Select Move Twist Add Erase Edit bonds Edit charges Add folder Add rings Periodic table Assets +H Add hydrogens +H Add H by res. type -H Remove hydrogens Store

History Clipboard Edit Snapping Add Adjust Conformations

2AZ8 - Dock animation.sa Selection filter Atoms and bonds Quick access

Search nodes... (Ctrl+) Look in All nodes

- 2AZ8
- 2AZ8-IA
- 2AZ8-IA
- 2AZ8-IB
- Ribbons 1
- How to create a dock animation
- AutoDock Vina Ext. - 2022-09-26
 - Configuration
 - 2AZ8 - Flexible residues
 - 2AZ8 - Flexible side chains
 - 2AZ8-IA - Initial conformation
 - 2AZ8-IA - Mode 1 (-8.6 kcal/m)**
 - 2AZ8-IA - Mode 2 (-8.5 kcal/m)
 - 2AZ8-IA - Mode 3 (-8.2 kcal/m)
 - 2AZ8-IA - Mode 4 (-7.9 kcal/m)
 - 2AZ8-IA - Mode 5 (-7.6 kcal/m)
 - 2AZ8-IA - Mode 6 (-7.3 kcal/m)
 - 2AZ8-IA - Mode 7 (-7.1 kcal/m)
 - 2AZ8-IA - Mode 8 (-6.9 kcal/m)
 - 2AZ8-IA - Mode 9 (-6.9 kcal/m)
 - 2AZ8-IA - Mode 10 (-6.8 kcal/r)

Current selection: 2AZ8-IA - Mo

Saved the selection to C:/Users/IKENAGA-PC/Downloads/2022-09-26_17h43m45s/results/2AZ8-IA/Initial conformation.mol2

AutoDock Vina Extended

Home Dock Results Log

Filter results: All results

Remove selected modes Remove hidden modes

mode	affinity (kcal/mol)	Ki (umol)	RMSD, lower bound (A)	RMSD, upper bound (A)
1	-8.57795	0.515605	0	0
2	-8.49476	0.593335	2.90623	4.48703
3	-8.18872	0.994545	2.21415	3.03261
4	-7.85444	1.74846	3.32792	6.1997
5	-7.63496	2.53244	2.82667	4.39614

Export table in CSV Tip: right-click on the table for additional functionality.

Plot

Color palette: Qualitative: Default Show ligand names

Font... Save image Export as csv

Affinity, kcal/mol

Compounds

計算結果一覧が表示されます。また、出力された各データをクリックすることで、それぞれのドッキングポーズを表示できます。

Protein-Ligand Interaction Analyzer

Setup | Surrounding residues | H-bonds

1 - Setup system

Receptor: Set Unset Select
Ligand: Set Unset Select

2 - Setup analysis

SASA probe radius: 0,14 Å
Surrounding residues cutoff radius: 5,00 Å

Hydrogen bonds between receptor and ligand

Cutoff distance: 3,50 Å | D-H...A angle ≥: 120°

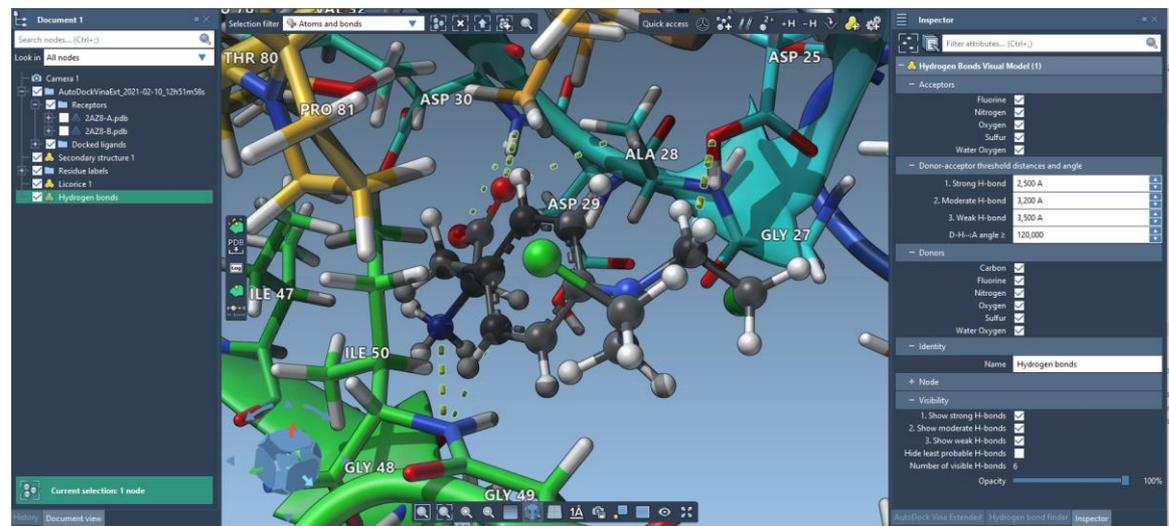
Donors: C N O F S
Acceptors: N O F S

3 - Analyze

Analyze: 100%

Asphericity	0,2045
H-bonds	6
Receptor's Rgyr (nm)	1,7483
System's Rgyr (nm)	1,7503
Receptor's SASA (nm ²)	229,675
Ligand's SASA (nm ²)	3,4573
System's SASA (nm ²)	231,638
Contact area (nm ²)	0,747

Export in csv



ドッキング結果を用いて、受容体-リガンド間の接触面積の算出や、水素結合を表示することなどが可能です。
また、有償アドオンにより、リガンド解離パスウェイの探索も可能です。

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