

SAMSON connect上 でのタンパク質構造予測 (ESMFold / AlphaFold)

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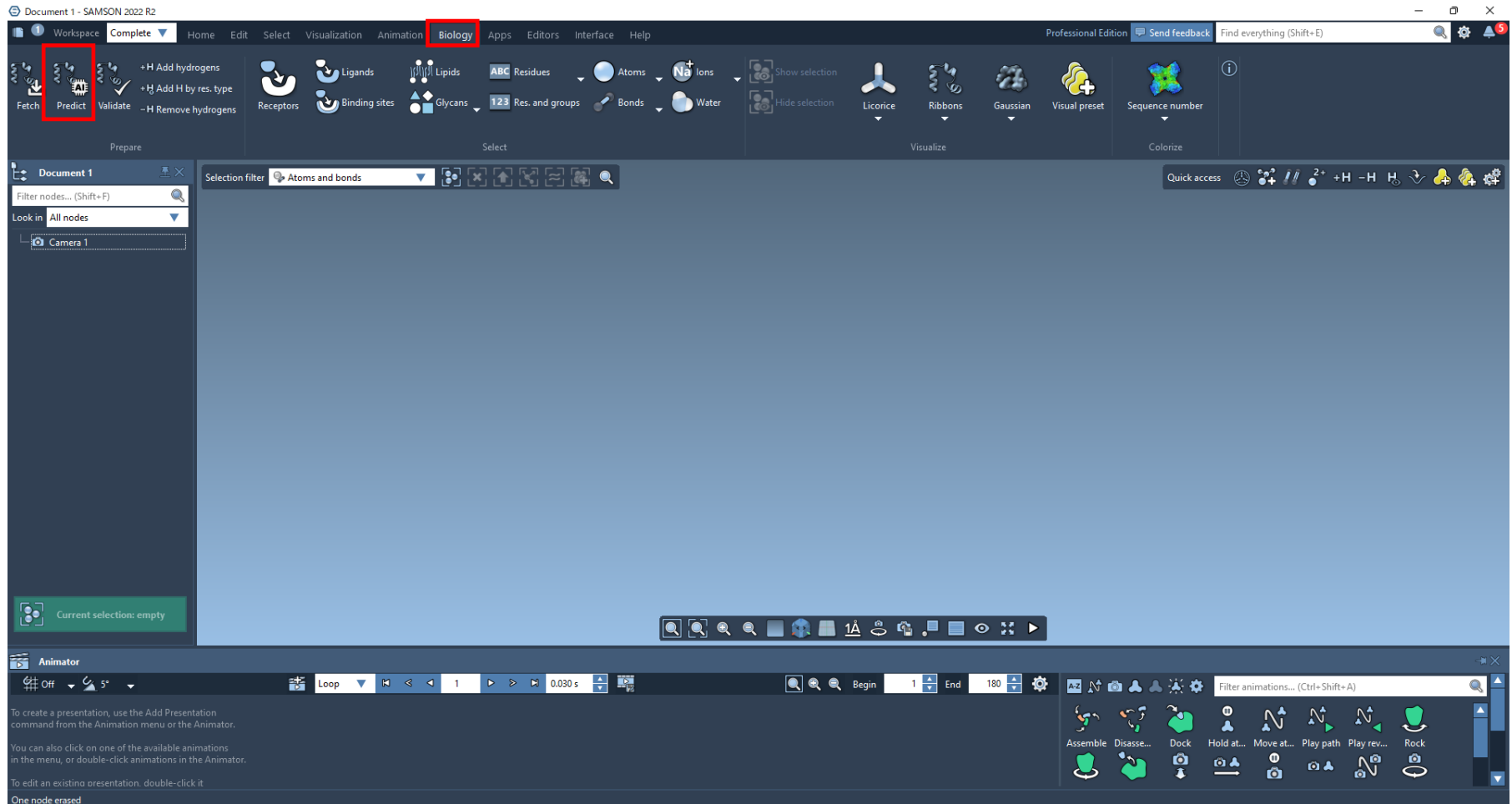


**今回は、ジャガイモ *Solanum tuberosum* 由来の
カルモジュリンのアミノ酸配列を使用しました。
(NP_001275359.1, 149アミノ酸)**

ESMFoldを用いた予測

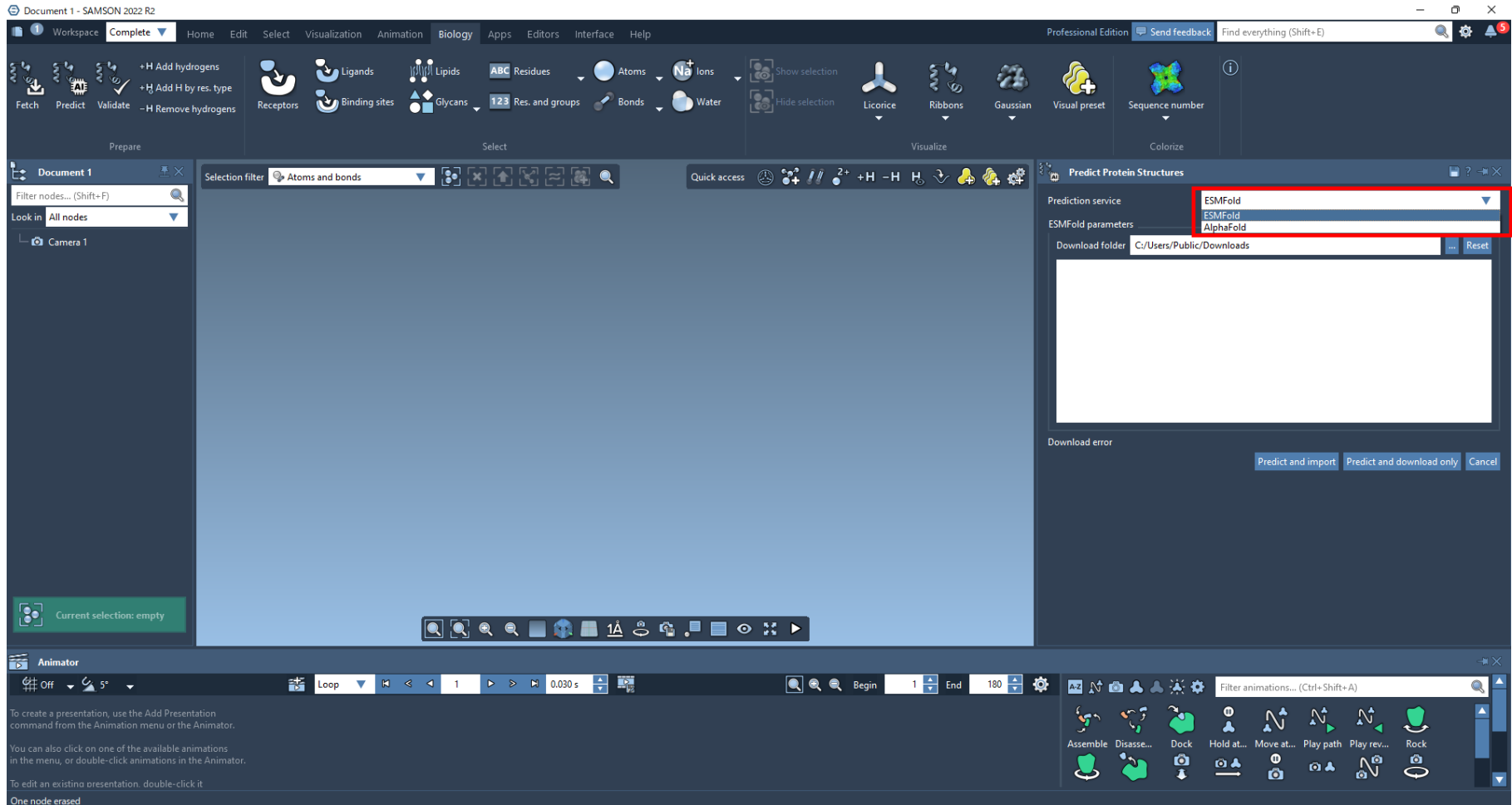
AlphaFoldを用いた予測

構造予測ツールの起動



Biologyタブを選択し、“Predict”をクリックします。

ESMFoldを選択



Prediction serviceメニューから“ESMFold”を選択します。

アミノ酸配列の入力

The screenshot displays the SAMSON 2022 R2 software interface. The main window is titled 'Document 1 - SAMSON 2022 R2'. The top menu bar includes 'Workspace', 'Complete', 'Home', 'Edit', 'Select', 'Visualization', 'Animation', 'Biology', 'Apps', 'Editors', 'Interface', and 'Help'. The top toolbar contains various icons for 'Fetch', 'Predict', 'Validate', 'Add hydrogens', 'Add H by res. type', 'Remove hydrogens', 'Receptors', 'Ligands', 'Binding sites', 'Lipids', 'Glycans', 'Res. and groups', 'Bonds', 'Water', 'Show selection', 'Hide selection', 'Licorice', 'Ribbons', 'Gaussian', 'Visual preset', 'Sequence number', and 'Colorize'. The left sidebar shows 'Document 1' with a 'Filter nodes...' search bar and a 'Look in' dropdown set to 'All nodes'. The main workspace is currently empty, with a 'Selection filter' set to 'Atoms and bonds'. The bottom status bar indicates 'Current selection: empty'. On the right, the 'Predict Protein Structures' panel is open, showing 'Prediction service' set to 'ESMFold'. Below this, the 'ESMFold parameters' section includes a 'Download folder' field set to 'C:/Users/Public/Downloads' and a 'Reset' button. A text area contains the amino acid sequence:
MADQLTEDQISEFKEAFSLFDKDGDCITTKELGTVMRSLGQNPTEAELQDMINEVDADNGTIDFPEFLNLMARK
MKDTSSEELKEAFRFDKDQNGFISAAELRHVMTNLGEKLTDEEVDREIADVDGQINVDYEFVKVMMAK
At the bottom of this panel, the 'Predict and import' button is highlighted with a red box. The bottom of the interface features an 'Animator' panel with a timeline and various animation controls.

コピー＆ペーストでアミノ酸配列を入力し、
“Predict and import”をクリックします。

結果の表示

The screenshot displays the SAMSON 2022 R2 software interface. The main window shows a 3D ribbon representation of a protein structure, colored by residue type (blue for helix, green for sheet, yellow for loop). The interface includes a top menu bar with options like Workspace, Complete, Home, Edit, Select, Visualization, Animation, Biology, Apps, Editors, Interface, and Help. A toolbar on the left contains icons for Fetch, Predict, Validate, and various molecular editing tools. A central panel shows the protein structure. On the right, a 'Predict Protein Structures' panel is active, displaying the ESMFold prediction service. It shows the ESMFold parameters, a download folder path, and a protein sequence: MADQLTDDQISEFKEAFSLFDKDGCGITTKELGTVMRLGQNPTEALQDMINEVDADGNGTIDFPEFLNLMARK MKDSTDSEELKEAFRVFDKQNGFISAAELRHVMTNLGKLTDEEVDEMIREADVDDGQINVDYFVKVMMMAK. The status is 'OK', and buttons for 'Predict and import', 'Predict and download only', and 'Cancel' are visible. At the bottom, an 'Animator' panel shows animation controls and a list of available animations.

Document 1 - SAMSON 2022 R2

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

Professional Edition Send feedback Find everything (Shift+E)

Fetch Predict Validate +H Add hydrogens +H Add H by res. type -H Remove hydrogens

Receptors Ligands Lipids Residues Atoms Na Ions Show selection Hide selection

Prepare Select Visualize

Selection filter Atoms and bonds

Quick access

Document 1

Filter nodes... (Shift+F)

Look in All nodes

Camera 1

ESM1

Receptor - Ribbons

Current selection: empty

Predict Protein Structures

Prediction service ESMFold

ESMFold parameters

Download folder C:/Users/Public/Downloads

MADQLTDDQISEFKEAFSLFDKDGCGITTKELGTVMRLGQNPTEALQDMINEVDADGNGTIDFPEFLNLMARK MKDSTDSEELKEAFRVFDKQNGFISAAELRHVMTNLGKLTDEEVDEMIREADVDDGQINVDYFVKVMMMAK

Status: OK

Predict and import Predict and download only Cancel

Animator

Off 5°

Loop

1 0.030 s

Begin 1 End 180

Filter animations... (Ctrl+Shift+A)

Assemble Disassemble Dock Hold at... Move at... Play path Play rev... Rock

To create a presentation, use the Add Presentation command from the Animation menu or the Animator.

You can also click on one of the available animations in the menu, or double-click animations in the Animator.

To edit an existing presentation, double-click it.

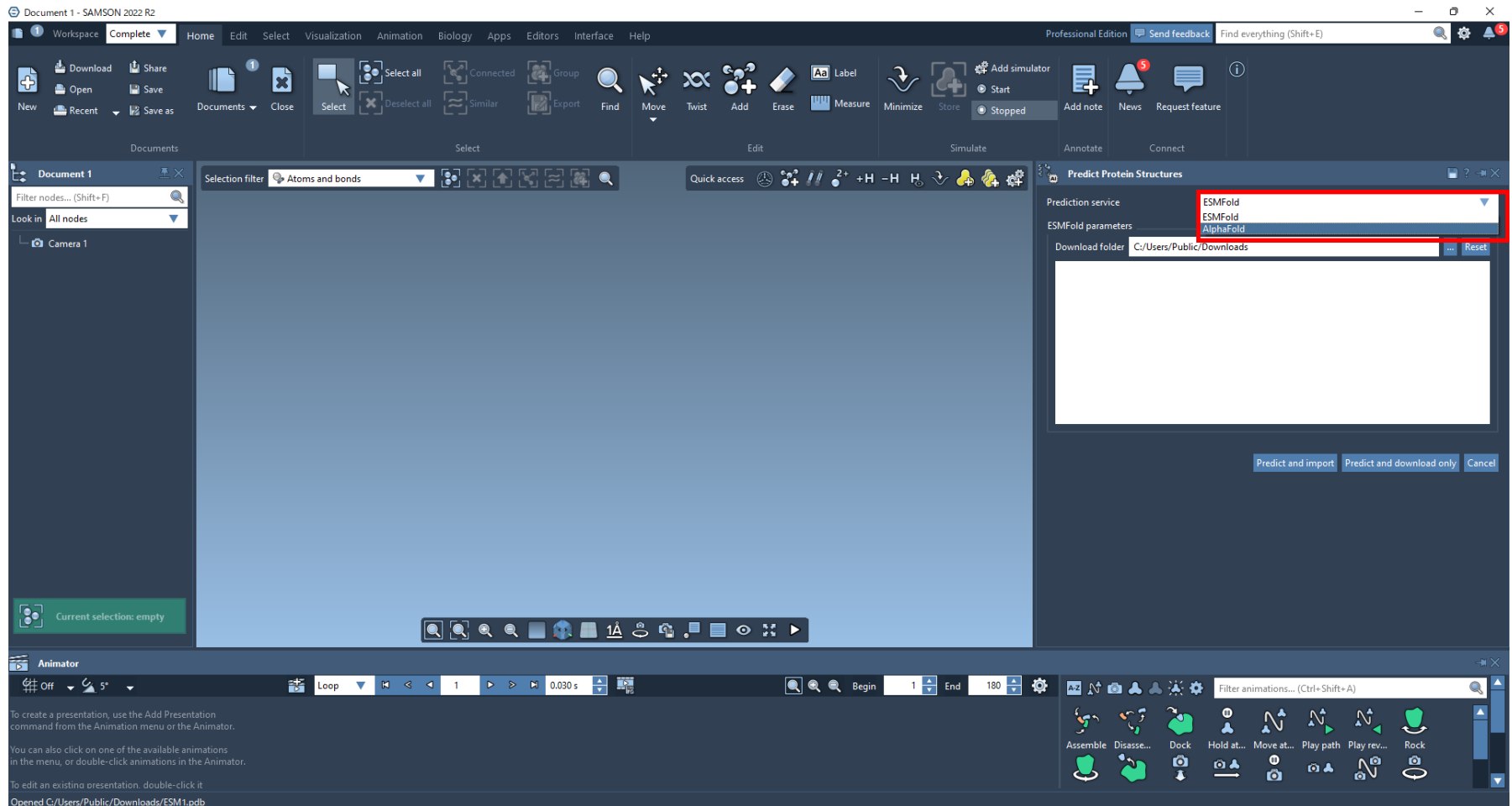
Opened C:/Users/Public/Downloads/ESM1.pdb

予測結果の構造データがインポートされます。
処理にかかった時間は1秒ほどでした。

ESMFoldを用いた予測

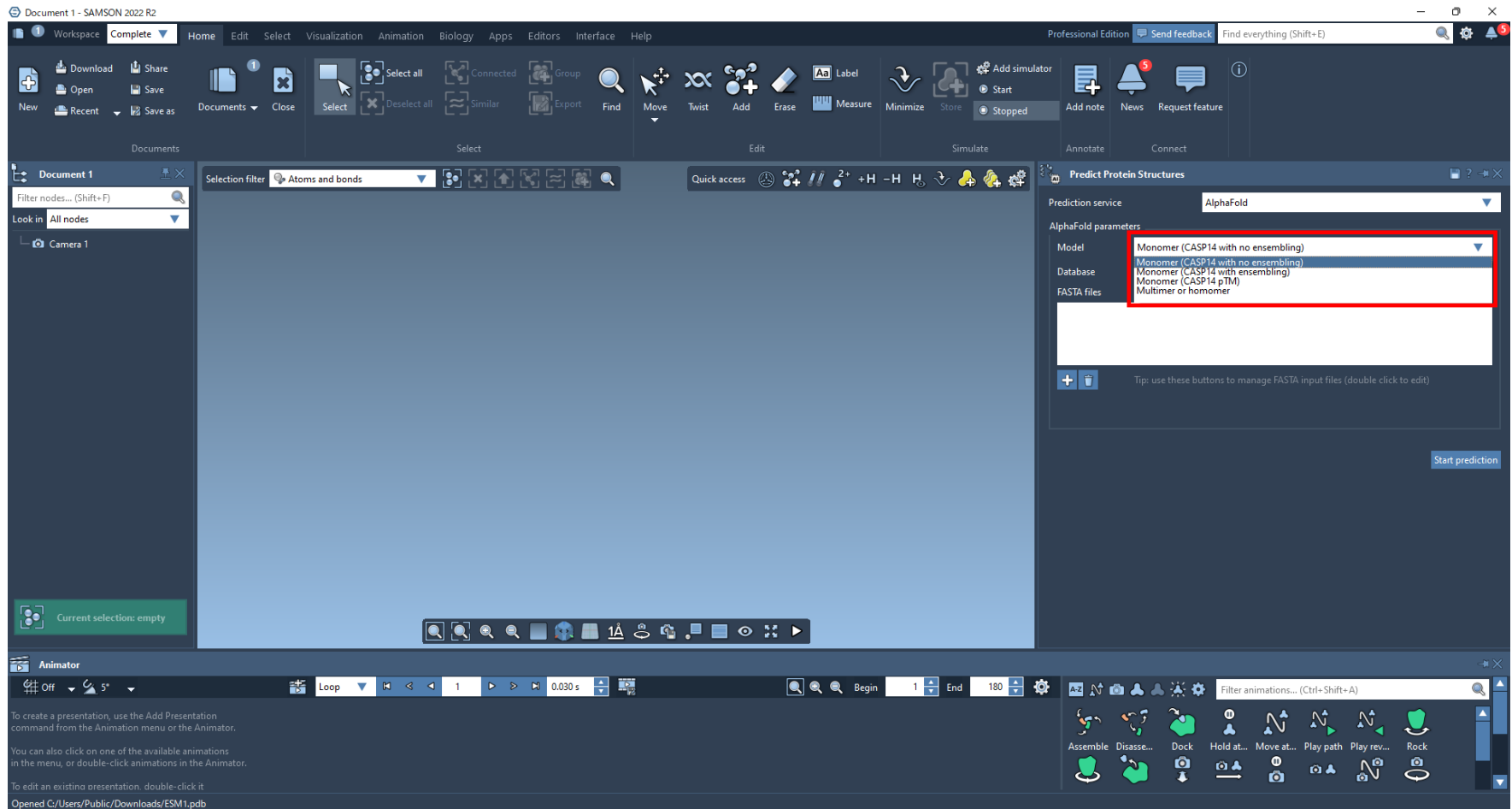
AlphaFoldを用いた予測

AlphaFoldを選択



Prediction serviceメニューから“AlphaFold”を選択します。

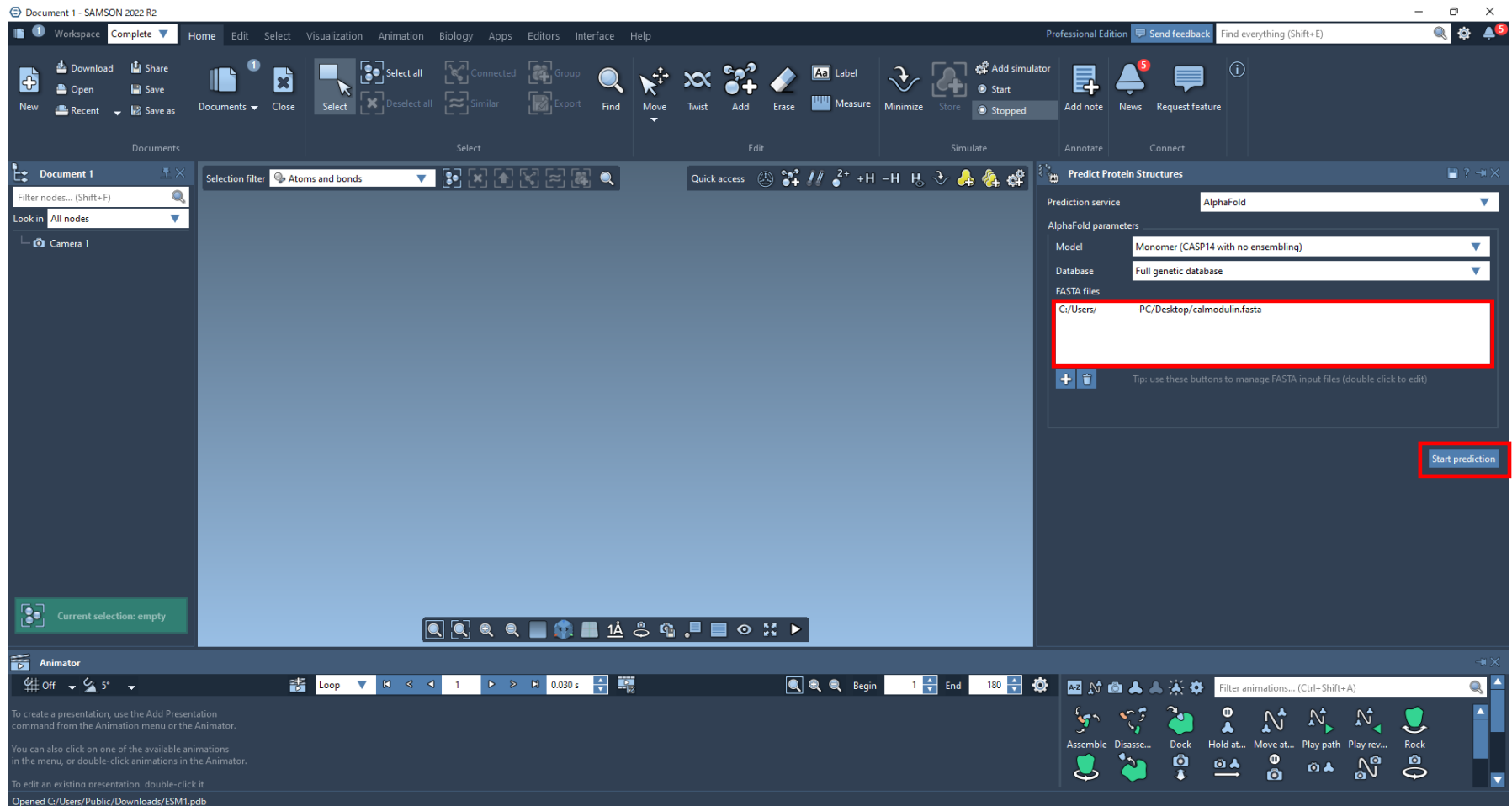
パラメーターの指定



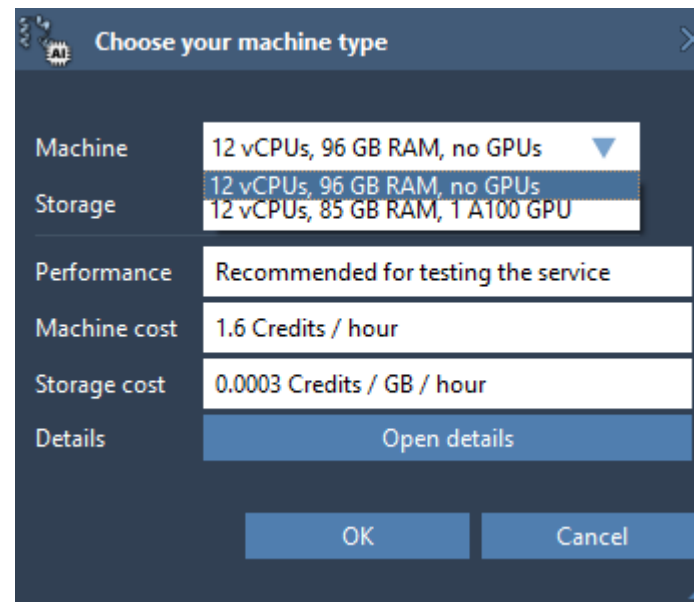
パラメーターを選択します。

複合体予測の際は、ここで“Multimer and homomer”を選択します。

ファイルの指定



アミノ酸配列のFASTAファイルを指定し、“Start Prediction”をクリックします。



計算に使用するマシンを選択します。
今回は上の12 vCPUs, 96GB RAM, no GPUsというマシンを使用しました。

The screenshot displays the SAMSON 2022 R2 software interface. The main window shows a molecular structure visualization. In the bottom-left corner, the 'Job manager' panel is visible, listing various jobs. One job, 'Alpha fold ...', is highlighted with a red box, indicating it is 'Completed' on '2022/12/07 7:54'. To the right, the 'Job files' window is open, showing the results of the job. It lists various output files (pdb, pickle, JSON) and their download status. The 'Download selection' and 'Download all' buttons are highlighted with red boxes. The 'Predict Protein Structures' panel on the right shows the 'AlphaFold' prediction service settings.

Job manager

Name	Status	Date created
Simulation of ...	Completed	2022/10/07 7:11
NVT equilibrati...	Completed	2022/10/07 1:35
NVT equilibrati...	Completed	2022/10/06 5:54
NPT equilibrati...	Completed	2022/10/07 1:52
NPT equilibrati...	Failed	2022/10/07 0:18
NPT equilibrati...	Cancelled	2022/10/06 8:59
Alpha fold ...	Completed	2022/12/07 7:54
Alpha fold ...	Running	2022/12/09 2:47

Job files

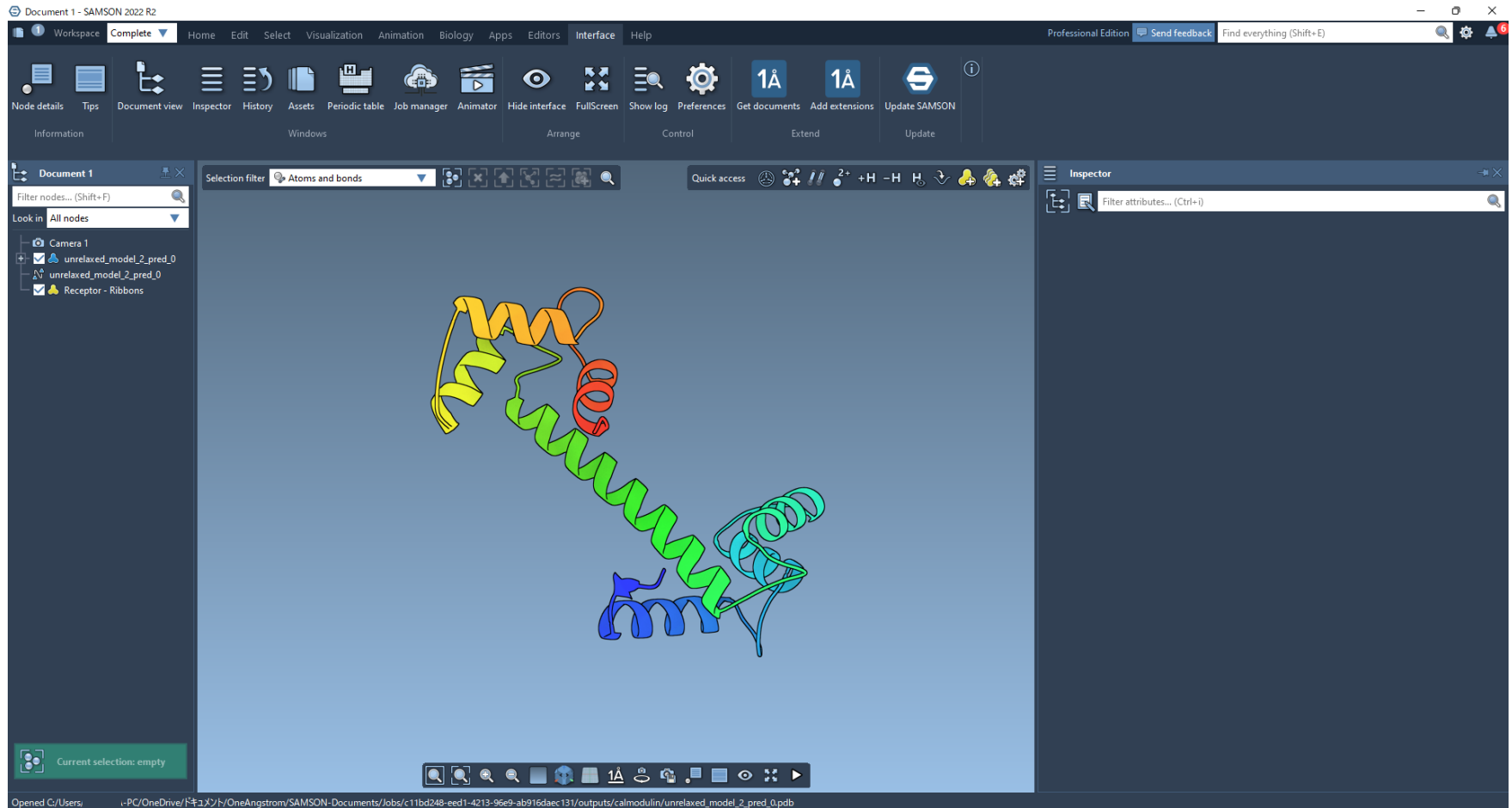
Results files of job: Alpha fold calculations | a512e165-428f-4a83-ae5f-ad02cdfa351d

Download folder: C:\Users\Public\OneDrive\OneAngstrom\SAMSON-Documents\Jobs\ [X] group downloads by job [Copy]

[Select all] [Download selection] [Download all]

File	Description	Size	Download status
outputs/...	pdbe file	713 kB	Not downloaded or not in the current specified path
outputs/...	pdbe file	713 kB	Not downloaded or not in the current specified path
outputs/...	pdbe file	713 kB	Not downloaded or not in the current specified path
outputs/...	pdbe file	713 kB	Not downloaded or not in the current specified path
outputs/...	pdbe file	713 kB	Not downloaded or not in the current specified path
outputs/...	A JSON format ...	873 B	Not downloaded or not in the current specified path
outputs/...	A pickle file	384 MB	Not downloaded or not in the current specified path
outputs/...	A pickle file	384 MB	Not downloaded or not in the current specified path
outputs/...	A pickle file	384 MB	Not downloaded or not in the current specified path
outputs/...	A pickle file	384 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	pdbe file	1 MB	Not downloaded or not in the current specified path
outputs/...	A JSON format ...	399 B	Not downloaded or not in the current specified path

計算が終了すると、登録済みのメールアドレスに通達されます。
Job managerより、出力ファイルの中から必要なものをダウンロードできます。



ダウンロードされた構造データをインポートします。
今回の処理にかかった時間は、2時間20分でした。

- 分子モデリング/シミュレーション用ソフトウェアSAMSON connectでは、タンパク質構造予測AI（ESMFold・AlphaFold）を用いた構造予測が可能です。
- アミノ酸配列を用意するだけで、簡単に予測が可能です。
- ESMFoldで予測する場合は、ローカル環境で計算が行われます。
- AlphaFoldで予測する場合は、クラウド環境で計算が行われるため、データベースのダウンロードや、高スペックPCの準備が不要です。
（※計算にはクラウドコンピューティングクレジットが必要です。）

製品HP: <https://filgen.jp/Product/BioScience21-software/OneAngstrom/index.html>

製品YouTube: <https://www.youtube.com/watch?v=reRD38RTI6E>

 SAMSON Connect

 OneAngstrom

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