DATA MANAGEMENT AND SHARING PLAN

Element 1: Data Type

A. Types and amount of scientific data expected to be generated in the project:

No	Type	Sample	Platform	Amount
(1)	Chromatography and Octet binding assay data	Receptor and antibody complexes	Exported as CSV files (Cytiva FPLC and Shimadzu HPLC)	~200 MB maximum
(2)	Radioligand binding and uptake assays	AMPA and NMDA receptor 3H binding experiments	Exported as CSV files from Perkin Elmer MicroBeta2	~20 MB maximum
(3)	Cryo-EM	AMPA and NMDA receptor, single particle; lamella tilt-series and tomograms	Glacios and Krios microscopes; exported as TIFF or MRC or EER	~500 TM maximum
(4)	Electrophysiology	GluA4 patch-clamp experiments	Exported as CSV files from pClamp	~10 MB maximum

B. Scientific data that will be preserved and shared, and the rationale for doing so:

All data described in A will be preserved and shared through public repositories to enable its easy reuse and analysis.

In addition, we will provide relevant detailed, step-by-step protocols data upon request. The methods that we develop to produce antibody fragments labeled with small gold nanoparticles (AuNPs) will be shared with the community and will be made available via a hyperlink on the lab's web page. All methods associated with new purification protocols will similarly be made available and, as usual, we will answer all inquiries quickly and thoroughly, aiming to help all interested parties make the most of our funded studies.

Material transfers will be made with no more restrictive terms than in the Simple Letter of Agreement (SLA) or the Uniform Biological Material Transfer Agreement (UBMTA) and without reach-through requirements. Should any intellectual property arise which requires a patent, we will ensure that the technology (materials and data) remains widely available to the research community in accordance with the NIH Principles and Guidelines document.

C. Metadata, other relevant data, and associated documentation:

To allow for the facile reuse and interpretation of the data, a README file and data directory will be created and deposited into an accessible repository, together with all shared data sets. The README file will include method description, instrument settings, and RRIDs of all relevant resources. The data directory will define and describe all variables in the data set.

All single particle cryo-EM data will be deposited in the Protein Data Bank (PDB; atomic coordinate data) and in the Electron Microscopy Data Bank (EMDB; electron microscopy data). Additional data will include half maps for data resolution calculation and masks used for map refinement. All cryo-ET data will be deposited in the Electron Microscopy Data Bank (EMDB; subtomogram averages and aligned tomograms) and Electron Microscopy Public Image Archive (EMPIAR; raw electron microscopy data).

Element 2: Related Tools, Software and/or Code

The chromatography and radioligand binding and uptake data will be stored as csv files and can be opened and managed using spreadsheet-based software or other common statistical analysis programs, such as R. The data from the computational studies will be in the form of either PDB files, visualized by Coot, ChimeraX or Pymol, and docking scores and MD analyses, readable by all commonly available word processing software. Cryo-EM images and movies can be viewed and processed using the freely available software packages that include RELION, Cryo-Sparc, and cisTEM. The cryo-EM maps and tomograms can be viewed using Coot, ChimeraX, and IMOD, all of which are freely available.

The electrophysiology data can be viewed and processed using the widely available pClamp software or imported into Graphpad Prism or other statistical analysis software for further processing.

Element 3: Standards

No consensus standards exist for the biophysical studies that include the radioligand binding experiments and the electrophysiological data. Nevertheless, all of our data and related methods will be described and organized adhering to best practices and in accordance with FAIR Principles for data. Unless where noted, all data will adhere to community standard file formats.

For the radioligand binding and electrophysiology data all experiments will be carried out at least 3 separate times, with 3 replicates each, data pooled and analyzed and fit to appropriate statistical functions.
The cryo-EM data will adhere to the standards put forth by the Protein Data Bank and the Electron Microscopy Data Bank. All cryo-EM data will be collected at well documented cryo-EM centers that regularly carry out benchmarking of the microscopes and the cameras, thus ensuring that pixel sizes and magnification values are correct. All resulting molecular models will be analyzed using Molprobity and also visually inspected using Coot, in order to make sure that the models have excellent stereochemistry. All models and maps will also be thoroughly inspected before deposition to the PDB and the EMDB. Data will be shared according to the standards established by the EMDB, EMPIAR, and PDB repositories.

Element 4: Data Preservation, Access, and Associated Timelines

A. Repository where scientific data and metadata will be archived:

Data will be carefully curated and along with relevant protocols, be deposited into FigShare+, where the items will be hosted for a minimum of 10 years. As is customary, all PDB files and EM density maps will be deposited with the PDB and the EMDB. We will link the relevant PDB and EMDB files with their places or elements in the protocols deposited into FigShare+.

B. How scientific data will be findable and identifiable:

FigShare provides searchable study-level metadata for dataset recovery. FigShare also assigns DOIs as identifiers and includes a strategy to preserve and ensure access over the long term. Data will be discoverable online through standard web search of the study-level metadata as well as the pointer from the DOI of the dataset. All publications and RPPRs will harbor the DOIs.
As is the field standard, the protein coordinates and density maps will have unique identifiers provided by the PDB and EMDB, respectively, and these identifiers will be included in all publications and RPPRs.

C. When and how long the scientific data will be made available:

The shared data will be made available as soon as the related work is published, or at the end of the grant period, whichever comes first. The shared data will be available for at least 5 years after the funding period ends.

Element 5: Access, Distribution, or Reuse Considerations

A. Factors affecting subsequent access, distribution, or reuse of scientific data:

The PI sees no factors or situations where all of the data derived from the present study will affect the access, distribution, or reuse of the data generated.
Related to the small molecule compounds developed under Aim 2, we emphasize that small quantities of the newly synthesized molecules will be made available at no cost to other researchers in the field, upon reasonable request. Analytical and spectral data supporting the identity and purity of the compound will be supplied with the sample.

B. Whether access to scientific data will be controlled:

There will be no controlled access – all data will be available immediately and will not require any approval.

C. Protections for privacy, rights, and confidentiality of human research participants:

No human data will be collected.

Element 6: Oversight of Data Management and Sharing

The PI for the proposed project, Dr. James Eric Gouaux, will make sure that all researchers associated with the project adhere to the Data Management and Sharing Plan (DMSP). Compliance will be monitored and reported in the annual Research Performance Progress Report (RPPR), which will include identification codes for data submitted to databanks and repositories.
The Office of Proposal and Award Management (OPAM) at Oregon Health & Science University, which will be administering this award, has created a data management and sharing plan compliance system as part of their process for submitting the annual (RPPR) to the National Institute of Neurological Disorders and Stroke (NINDS). OPAM will secure certification from the PI that the DMSP is compliant as approved. If the PI cannot certify compliance, OPAM will work with the team to ensure non-compliance is adequately addressed.