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Reporting Summary

Nature Portfolio wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Portfolio policies, see our <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

Statistics

For	all st	atistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.
n/a	Cor	firmed
	\square	The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement
	\square	A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
		The statistical test(s) used AND whether they are one- or two-sided Only common tests should be described solely by name; describe more complex techniques in the Methods section.
	\boxtimes	A description of all covariates tested
	\boxtimes	A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
	\boxtimes	A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
		For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted Give <i>P</i> values as exact values whenever suitable.
\boxtimes		For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
\boxtimes		For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
	\boxtimes	Estimates of effect sizes (e.g. Cohen's d, Pearson's r), indicating how they were calculated
	1	Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.

Software and code

Policy information	about <u>availability of computer code</u>
Data collection	enigmatoolbox v1.1.1 (https://github.com/MICA-MNI/ENIGMA) was used for fetching ENIGMA data. MEG data was processed using the open software toolbox Brainstorm v220420. HCP structural data was processed using MRtrix3 v3.0.0
Data analysis	All code used to analyze data can be found at https://github.com/netneurolab/hansen_receptors. Data was analyzed using Python 3.8.10, MATLAB R2022a, netneurotools v0.2.3 and neuromaps v0.0.3.

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio guidelines for submitting code & software for further information.

Data

Policy information about availability of data

All manuscripts must include a data availability statement. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our policy

All data used to perform the analyses can be found at https://github.com/netneurolab/hansen_receptors. Volumetric PET images, including receptor images and synaptic density, are included in neuromaps (https://github.com/netneurolab/neuromaps) where they can be easily converted between template spaces. Autoradiography data is available in Supplementary Table 2 of Zilles & Palomero-Gallagher 2017, Frontiers in Neuroanatomy. The HCP dataset, including diffusion weighted MRI, fMRI, and MEG is available at https://db.humanconnectome.org/. Neurosynth data is available at https://neurosynth.org/. The ENIGMA datasets are

available through the ENIGMA consortium and the ENIGMA toolbox (https://github.com/MICA-MNI/ENIGMA). Parcellation atlases including the Schaefer-100 and Desikan-Killiany atlas were fetched from netneurotools (https://github.com/netneurolab/netneurotools).

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

Ecological, evolutionary & environmental sciences

Life sciences

Behavioural & social sciences

For a reference copy of the document with all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Sample size	No sample size calculations were performed. We collated as many PET tracer images as possible to construct a comprehensive (19-receptor/ transporter) atlas. HCP data was used because of the large number of subjects and the relatively equal male/female balance. For HCP data, only unrelated subjects were included. For PET data, only healthy subjects were included. The ENIGMA dataset was selected because of the large number of subjects in each meta-analysis and because it contains many brain maps for diseases/disorders/conditions that have been similarly processed such that comparison between datasets is possible.
Data exclusions	No data was excluded.
Replication	The analysis pipeline was conducted and replicated: (1) at the Schaefer-100 parcellation resolution, (2) at the Schaefer-200 parcellation resolution, (3) at the Schaefer-400 parcellation resolution, (4) using the 68-node Desikan Killiany atlas alongside structural/functional connectomes from the Lausanne atlas. Furthermore, we recalculated the receptor similarity matrix in a leave-one-out fashion, and confirmed that no single receptor/transporter exerts undue influence on this similarity matrix (correlation between leave-one-out similarity matrix and original similarity matrix >0.98 for all receptors). Finally, analyses were repeated using autoradiography data for 15 receptors as opposed to PET data for 19 receptors/transporters.
Randomization	No randomization was performed as this study does not include experimental groups.
Blinding	Blinding is not relevant to this study because it does not include experimental groups.

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

Methods

n/a	Involved in the study	n/a	Involved in the study	
\times	Antibodies	\boxtimes	ChIP-seq	
\ge	Eukaryotic cell lines	\ge	Flow cytometry	
\boxtimes	Palaeontology and archaeology		MRI-based neuroimaging	
\boxtimes	Animals and other organisms			
	Human research participants			
\square	Clinical data			

Human research participants

Dual use research of concern

Policy information about studies involving human research participants				
Population characteristics	Demographic information for all PET subjects can be found in Table 1.			
Recruitment	Only data from healthy control subjects were used in the analyses.			
Ethics oversight	Each individual PET study was approved, details can be found in the references found in Table 1.			

Note that full information on the approval of the study protocol must also be provided in the manuscript.

Magnetic resonance imaging

Experimental design	
Design type	Resting-state fMRI and diffusion-weighted MRI
Design specifications	Following the procedure described in Vos De Wael et al., 2018, we obtained structural and functional magnetic resonance imaging (MRI) data for 326 unrelated participants (age range 22–35 years, 145 males) from the Human Connectome Project (HCP; S900 release). All four resting state fMRI scans (two scans (R/L and L/R phase encoding directions) on day 1 and two scans (R/L and L/R phase encoding directions) on day 2, each about 15 min long; TR=720 ms), as well as diffusion weighted imaging (DWI) data were available for all participants. All the structural and functional MRI data were pre-processed using HCP minimal pre-processing pipelines. Detailed information regarding data acquisition and pre-processing is available elsewhere (Van Essen et al., 2013, Glasser et al., 2013)
Behavioral performance measures	No behavioural measures were recorded during the fMRI runs.
Acquisition	
Imaging type(s)	Functional and diffusion-weighted MRI
Field strength	3T

Sequence & imaging parameters	Multi-band sequence; functional images have a 2-mm isotropic signal resolution, structural modalities were acquired on a Siemens Skyra 3T scanner and included a T1-weighted MPRAGE sequence at an isotropic resolution of 0.7mm, and a T2-weighted SPACE at an isotropic resolution of 0.7mm. More details on imaging protocols and procedures are available at http://protocols.humanconnectome.org/HCP/3T/imaging-protocols.html.		
Area of acquisition	Whole-brain		
Diffusion MRI Used	Not used		
reprocessing			
Preprocessing software	We used the HCP data that was previously preprocessed. This preprocessing was done using FSL 5.0.6, FreeSurfer 5.3.0-HCP, and Connectome Workbench v1.1.1.		
Normalization	Image processing includes correcting for gradient distortion caused by non-linearities, correcting for bias field distortions, and registering the images to a standard reference space.		
Normalization template	fs_LR_32k surface mesh		
Noise and artifact removal	FMRIB's ICA-based X-noisefier (FIX) and global signal regression		
Volume censoring	No volume censoring was performed.		

Statistical modeling & inference

Model type and settings	Functional and structural connectomes were used for comparison with PET-derived receptor similarity.			
Effect(s) tested	We tested whether receptor similarity is greater when regions are connected (SC) or within the same intrinsic functional network (fMRI).			
Specify type of analysis: 🛛 Whole brain 🗌 ROI-based 🗌 Both				
Statistic type for inference (See <u>Eklund et al. 2016</u>)	NA			
Correction	NA			

Models & analysis

Ρ

n/a	Involved in the study				
	Functional and/or effective connectivity				
	Graph analysis				
	Multivariate modeling or predictive analysis				
Functional and/or effective connectivity		We used functional connectivity, which was constructed by correlated pairwise regional functional time series, and averaging this across subjects.			

We used structural connectivity (weighted) matrices. Structural connectivity between pairs of regions was