Supplemental Materials

In this section, we provide additional details and results related to the performance evaluation and analysis of the CAROT (Connectome Alignment using Robust Optimization and Topology) framework. The supplementary material encompasses various aspects, including the evaluation metrics used, parameter sensitivity analysis, optimal transport mappings, and the performance comparison based on different distance measures and nearest neighbor settings.

1. CAROT performance (i.e., in resting scans) using the Euclidean distance between the center of gravity for each ROI as the cost measure (see Fig. S1).

2. CAROT performance using Mean Squared Error (MSE) between original and reconstructed connectomes: The performance of the CAROT framework is assessed by quantifying the similarity between the original connectomes and the reconstructed connectomes. MSE is utilized as the evaluation metric, which measures the average squared difference between corresponding elements of the two matrices. The lower the MSE value, the higher the similarity between the original and reconstructed connectomes (see Fig. S2 and Tab. S2).

3. Parameter sensitivity analysis: To investigate the impact of different parameters on the CAROT framework, a parameter sensitivity analysis is conducted. Specifically, the sensitivity of frame size, training data, and entropy regularization parameter epsilon (ϵ) is examined. Multiple target atlases are considered, and the analysis aims to determine the optimal parameter values that yield the best alignment results (see Fig. S4).

4. Frobenius norm between reconstructed and original Connectomes: In addition to MSE, the similarity between the reconstructed and original connectomes is also assessed using the Frobenius norm. The Frobenius norm calculates the square root of the sum of squared differences between corresponding elements of the matrices. By computing the Frobenius norm for each source-target pair, a comprehensive evaluation of the alignment performance is achieved (see Fig. S3 and Tab. S1).

5. Optimal transport mappings derived from resting scans data: Examples of mappings used by CAROT to align connectomes from different atlases to a common target atlas, such as the Shen atlas (see Fig. S5).

6. MSE and Spearman correlation with KNN: To explore the impact of different distance measures and nearest neighbor settings on the alignment performance, MSE and Spearman correlation coefficients are calculated. The analysis is conducted for both k=1 (see Tab. S3 and Tab S5) and k=5 (see Tab. S4 and Tab. S6) nearest neighbor settings using both Euclidean distance and functional distance measures. The results are presented as mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

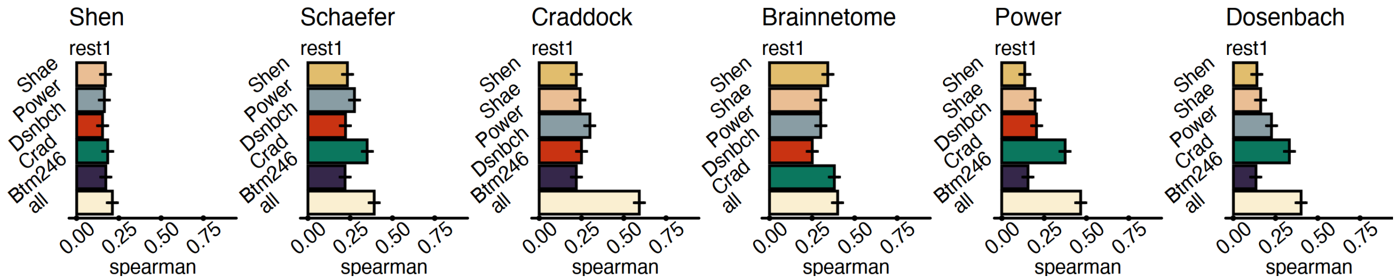


Fig. S1: CAROT performance (rest) using euclidean distance between the center of gravity for each ROI as the cost measure. The results exhibit significantly lower performance compared to functional distance.

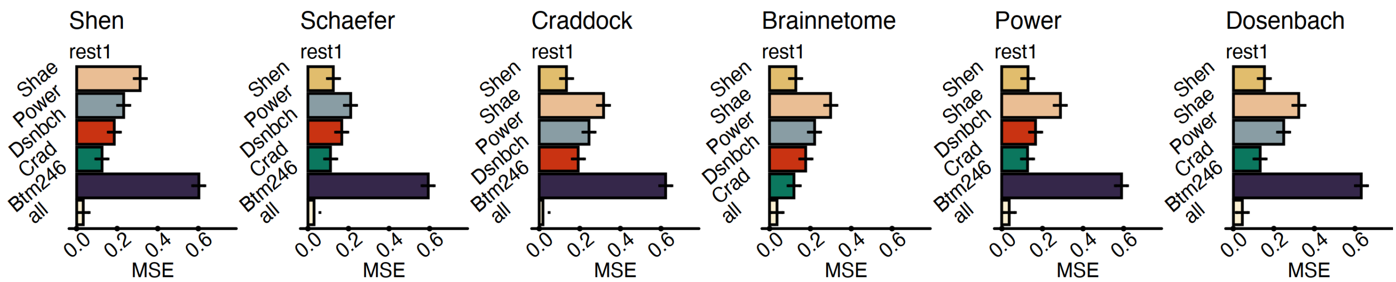


Fig. S2: CAROT performance using mean squared error (MSE) between original and reconstructed connectomes.

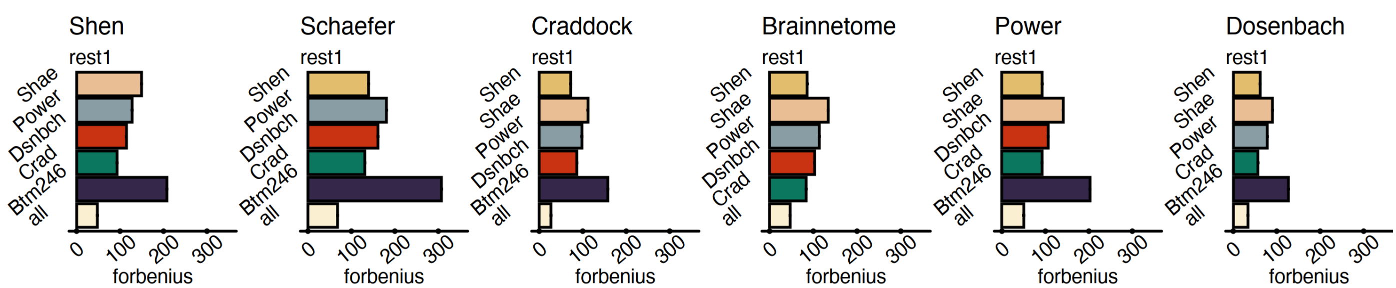
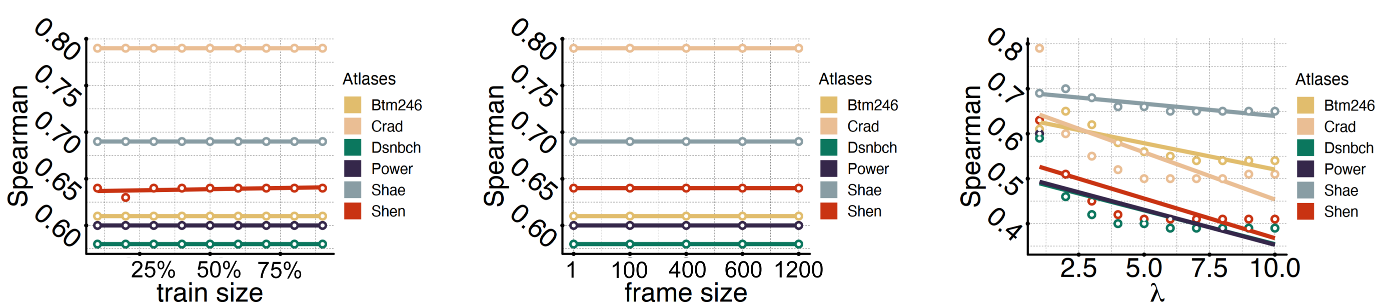


Fig. S3: CAROT performance using Frobenius distance between original and reconstructed connectomes.



(a) Train Size Sensitivity

(b) Frame Size Sensitivity

(c) Entropy Penalty

Fig. S4: Parameter sensitivity of frame size, training data, and entropy regularization ϵ for different target atlases.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		139.60 ± 0.681	72.03 ± 0.300	86.26 ± 0.428	92.67 ± 0.571	61.63 ± 0.189
Schaefer	149.24 ± 0.484		111.82 ± 0.251	133.76 ± 0.498	140.62 ± 0.461	90.51 ± 0.346
Craddock	93.05 ± 0.437	131.40 ± 0.773		83.61 ± 0.568	92.11 ± 0.441	57.10 ± 0.258
Brainnetome	207.67 ± 0.462	307.43 ± 0.667	157.73 ± 0.197		202.34 ± 0.328	127.02 ± 0.233
Power	127.68 ± 0.562	180.89 ± 0.528	97.94 ± 0.356	113.94 ± 0.531		78.76 ± 0.384
Dosenbach	114.29 ± 0.771	161.30 ± 0.714	86.88 ± 0.411	102.56 ± 0.430	106.23 ± 0.555	

Table S1: Frobenius norm between reconstructed connectomes and original connectomes for each source-target pair. Presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

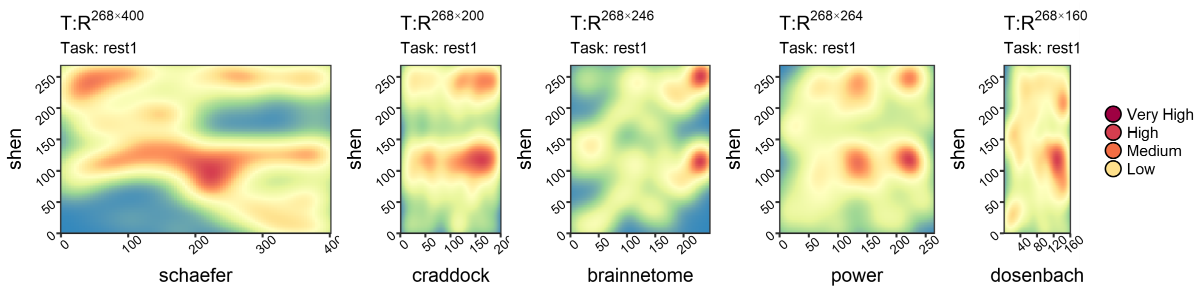


Fig. S5: Optimal transport mappings derived from resting data to the Shen atlas (target atlas) from each other atlas. The warmer color indicates regions that contribute the most towards mapping between atlases. Horizontal blue areas may indicate locations that are missing in the source atlas. For example, the Schaefer atlas does not include regions in the cerebellum, while the Shen does.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		0.126 ±0.001	0.13 ±0.001	0.12 ±0.001	0.12 ±0.001	0.15 ±0.001
Schaefer	0.31 ±0.002		0.31 ±0.00	0.30 ±0.002	0.29 ±0.002	0.32 ±0.002
Craddock	0.12 ±0.014	0.11 ±0.001		0.12 ±0.00	0.12 ±0.001	0.13 ±0.001
Brainnetome	0.60 ±0.003	0.59 ±0.002	0.62 ±0.001		0.59 ±0.002	0.63 ±0.002
Power	0.23 ±0.002	0.21 ±0.001	0.24 ±0.00	0.22 ±0.002		0.25 ±0.002
Dosenbach	0.19 ±0.003	0.17 ±0.002	0.19 ±0.002	0.18 ±0.002	0.17 ±0.002	

Table S2: Mean Sqaure error between reconstructed connectomes and original connectomes for each source-target pair. Presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		0.00 ±0.00	0.04 ±0.001	0.03 ±0.001	0.02 ±0.00	0.01 ±0.001
Schaefer	0.03 ±0.001		0.01 ±0.001	0.01 ±0.000	0.05 ±0.00	0.07 ±0.000
Craddock	0.06 ±0.000	0.02 ±0.000		0.02 ±0.00	0.17 ±0.000	0.23 ±0.000
Brainnetome	0.03 ±0.000	0.00 ±0.000	0.05 ±0.000		0.02 ±0.000	0.03 ±0.000
Power	0.05 ±0.000	0.00 ±0.000	0.19 ±0.001	0.00 ±0.000		0.16 ±0.002
Dosenbach	0.06 ±0.001	0.00 ±0.000	0.08 ±0.000	0.01 ±0.000	0.70 ±0.001	

Table S3: Spearman correlation between reconstructed connectomes and original connectomes for each source-target pair when using $k = 1$ nearest neighbor and Euclidean distance. The presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		0.02 ±0.001	0.06 ±0.001	0.06 ±0.001	0.04 ±0.001	0.03 ±0.001
Schaefer	0.04 ±0.001		0.18 ±0.001	0.06 ±0.00	0.09 ±0.001	0.14 ±0.001
Craddock	0.04 ±0.001	0.08 ±0.001		0.05 ±0.003	0.35 ±0.00	0.32 ±0.003
Brainnetome	0.04 ±0.001	0.01 ±0.001	0.06 ±0.001		0.05 ±0.001	0.04 ±0.001
Power	0.05 ±0.001	0.03 ±0.001	0.29 ±0.002	0.02 ±0.001		0.25 ±0.002
Dosenbach	0.05 ±0.000	0.012 ±0.002	0.21 ±0.001	0.02 ±0.001	0.15 ±0.002	

Table S4: Spearman correlation between reconstructed connectomes and original connectomes for each source-target pair when using $k = 5$ nearest neighbor and Euclidean distance. Presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		0.07 ±0.000	0.38 ±0.003	0.07 ±0.002	0.13 ±0.003	0.17 ±0.004
Schaefer	0.16 ±0.002		0.29 ±0.003	0.09 ±0.002	0.17 ±0.003	0.14 ±0.008
Craddock	0.23 ±0.002	0.09 ±0.002		0.11 ±0.002	0.17 ±0.002	0.20 ±0.005
Brainnetome	0.02 ±0.002	0.00 ±0.001	0.06 ±0.002		0.012 ±0.001	0.02 ±0.002
Power	0.08 ±0.002	0.03 ±0.002	0.18 ±0.003	0.03 ±0.004		0.17 ±0.005
Dosenbach	0.05 ±0.001	0.03 ±002	0.09 ±0.002	0.03±0.001	0.08 ±0.001	

Table S5: Spearman correlation between reconstructed connectomes and original connectomes for each source-target pair when using $k = 1$ nearest neighbor and functional distance. Presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.

	Shen	Schaefer	Craddock	Brainnetome	Power	Dosenbach
Shen		0.36 ±0.002	0.55 ±0.003	0.27 ±0.067	0.34 ±0.005	0.36 ±0.006
Schaefer	0.17 ±0.002		0.30 ±0.002	0.20 ±0.005	0.26 ±0.003	0.21 ±0.002
Craddock	0.41 ±0.004	0.39 ±0.007		0.31 ±0.005	0.37 ±0.005	0.38 ±0.011
Brainnetome	0.11 ±0.002	0.11 ±0.005	0.24 ±0.004		0.12 ±0.005	0.11 ±0.003
Power	0.14 ±0.003	0.27 ±0.005	0.33 ±0.003	0.18 ±0.004		0.27 ±0.004
Dosenbach	0.10 ±0.002	0.12 ±0.003	0.22 ±0.003	0.07 ±0.003	0.15 ±0.000	

Table S6: Spearman correlation between reconstructed connectomes and original connectomes for each source-target pair when using $k = 5$ nearest neighbor and functional distance. Presented results show mean ± standard deviation over 100 iterations of randomly splitting the data into training and testing sets.