Supplementary Materials for

Flexible brain transitions between hierarchical network segregation and integration predict human behavior

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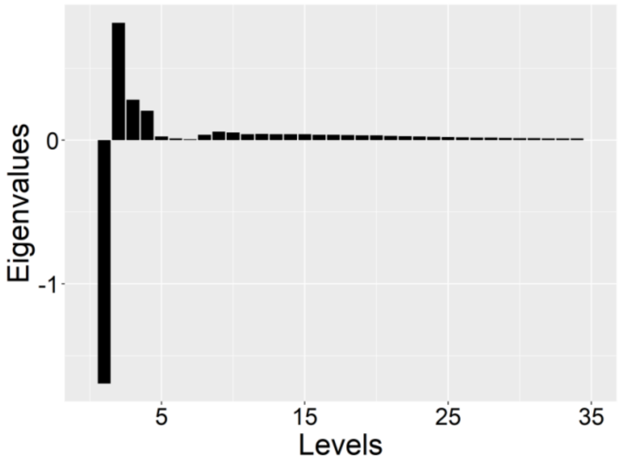
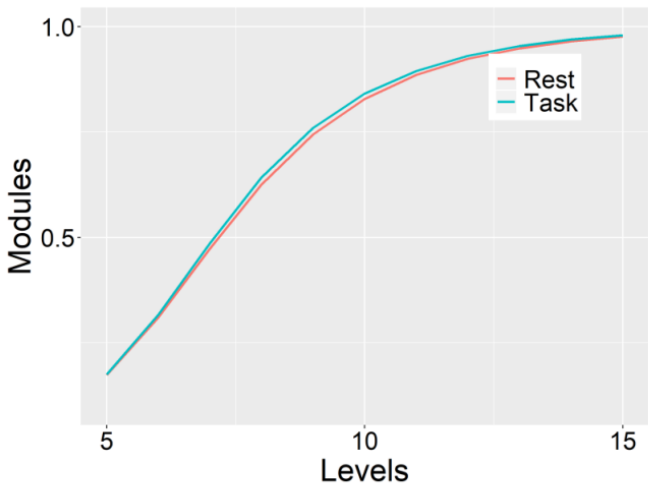
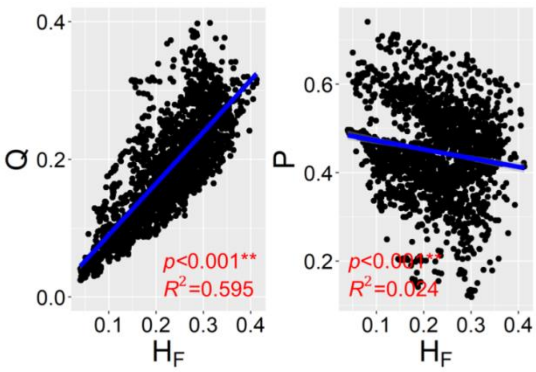
Supplementary Figures



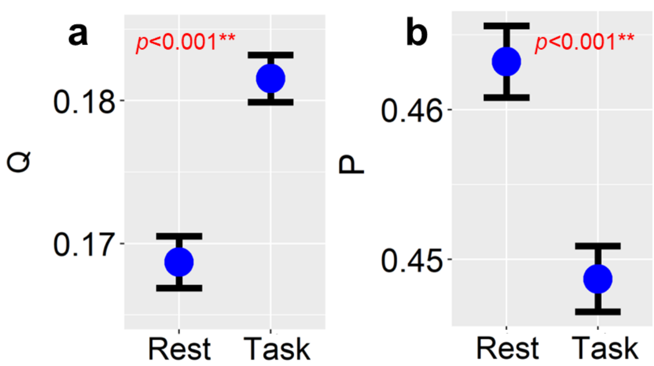
Supplementary Figure 1. Eigenvalue difference between task and resting states at each level. The largest eigenvalue corresponds to the first level and was significantly decreased in the task state, but the eigenvalues from the 2nd to 90th levels were increased.



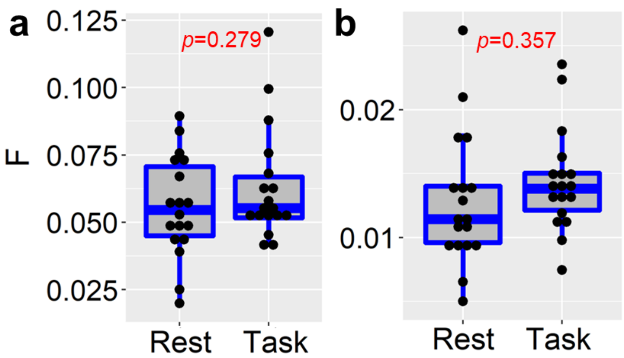
Supplementary Figure 2. More hierarchical modules in FC networks in the task state. The module number was normalized into [0, 1] by dividing *N*. A significant difference existed from the 5th to 19th levels.



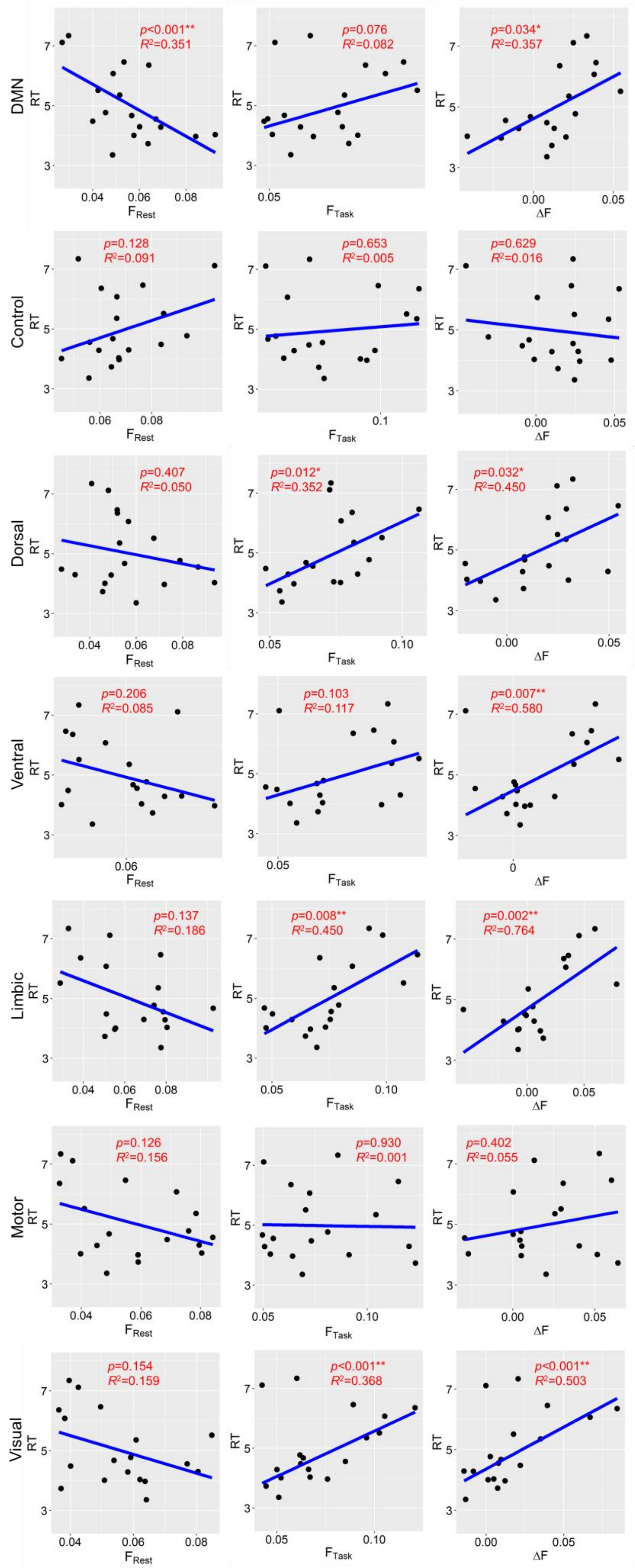
Supplementary Figure 3. H_F significantly related to graph-based network measures in the task state. These plots were calculated from all subjects and time windows. The significant correlations between H_F, modularity Q and participation coefficient P revealed that H_F based on hierarchical levels can capture the properties of brain FC networks, classically reflected by network measures based on one level. It should also be noted that Q and P vary much for a specific H_F, especially for large H_F, indicating that H_F may more effectively capture individual differences.



Supplementary Figure 4. Higher segregated processes in the task state measured by graph-based network measures. (a) Modularity Q and **(b)** participation coefficient P.

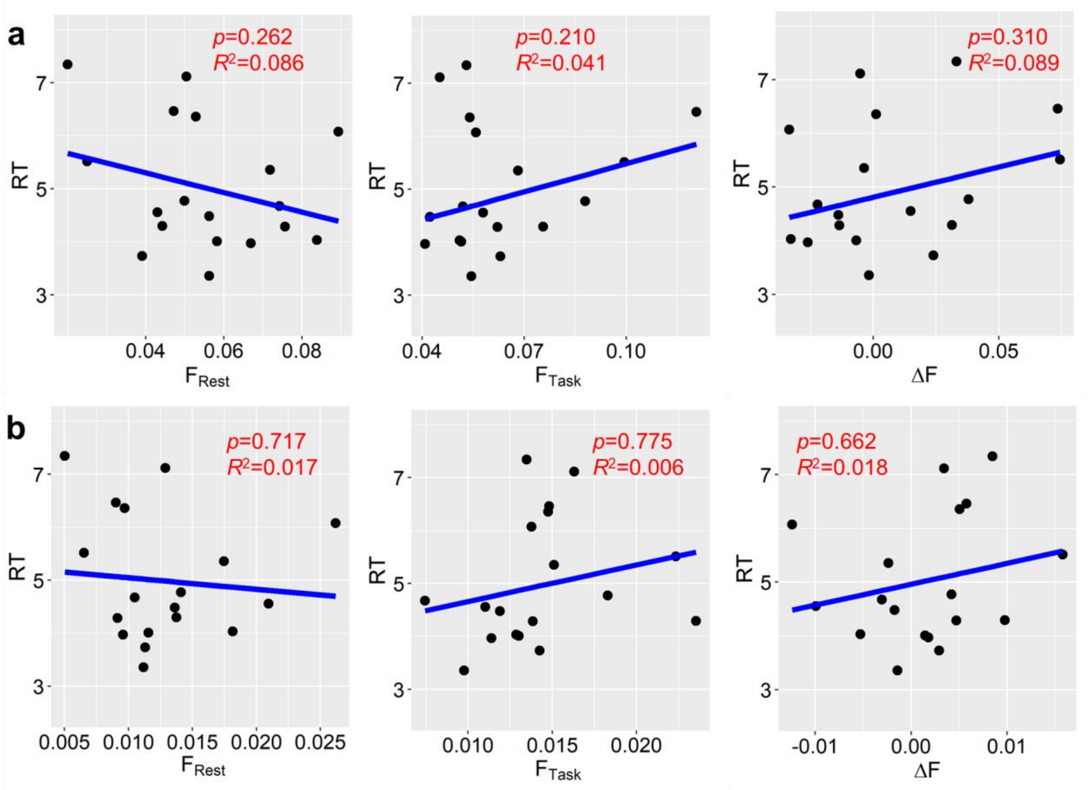


Supplementary Figure 5. Functional flexibility based on network measures was not sensitive to task. The functional flexibility was measured by the standard variance in **(a)** modularity Q and **(b)** participation coefficient P. The nonsignificant differences (two-sample t-test, $p>0.05$) in functional flexibility indicated that our method based on hierarchical modules in FC networks can capture more properties of dynamic functional organization than graph-based network measures at just one level.

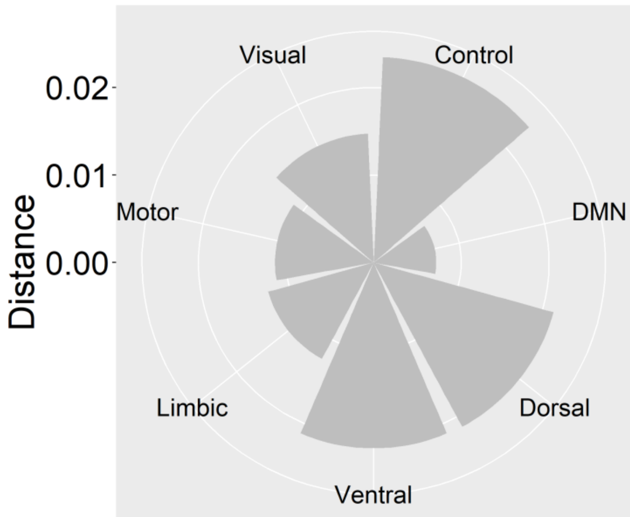


DMN
RT
FRest
FTask
ΔF
p<0.001**
R2=0.351
p=0.076
R2=0.082
p=0.034*
R2=0.357
Control
p=0.128
R2=0.091
p=0.653
R2=0.005
p=0.629
R2=0.016
Dorsal
p=0.407
R2=0.050
p=0.012*
R2=0.352
p=0.032*
R2=0.450
Ventral
p=0.206
R2=0.085
p=0.103
R2=0.117
p=0.007**
R2=0.580
Limbic
p=0.137
R2=0.186
p=0.008**
R2=0.450
p=0.002**
R2=0.764
Motor
p=0.126
R2=0.156
p=0.930
R2=0.001
p=0.402
R2=0.055
Visual
p=0.154
R2=0.159
p<0.001**
R2=0.368
p<0.001**
R2=0.503

Supplementary Figure 6. Correlation of functional flexibility with cognitive performance in different subsystems. Here, the *p*-values and R^2 were calculated from the robust linear regression, and *p*-values were further corrected.



Supplementary Figure 7. Functional flexibility based on graph-based network measures cannot predict cognitive performance. The functional flexibility was measured by the standard variance in **(a)** modularity Q and **(b)** participation coefficient P.



Supplementary Figure 8. The default mode network (DMN) may capture the main signature of the globally flexible transition between segregated and integrated states in the resting state. The intrinsic flexibility in the resting state was first calculated for all subjects, forming a vector $F = [F_1, \cdots, F_{18}]$. This vector exists in the whole-brain network and seven functional subsystems. We then calculated the distance between vectors for the whole-brain network and each of the functional subsystems. The DMN had the smallest distance to the whole-brain network, indicating that the DMN may capture the main signature of functional flexibility of the whole-brain.

Supplementary Tables

Supplementary Table 1. Residual standard error (SSE) in the robust linear regression between functional flexibility and task performance. Here, the functional flexibility was measured by the standard variance of H_F, modularity Q and participation coefficient P. It is apparently that the functional flexibility F_{Rest}, F_{Task} and ΔF based on hierarchical modules can robust predict task performance than that based Q and P, and the SSE based on hierarchical modules was also smaller than that based on Q and P. Thus, our method based on hierarchical modules in FC networks detected individual behavioral difference more effectively than the graph-based network measures at a single level.

SSE	Std. H_F	Std. Q	Std. P
F_{Rest}	0.774	1.302	1.346
F_{Task}	0.852	0.888	1.251
ΔF	0.463	0.973	1.526