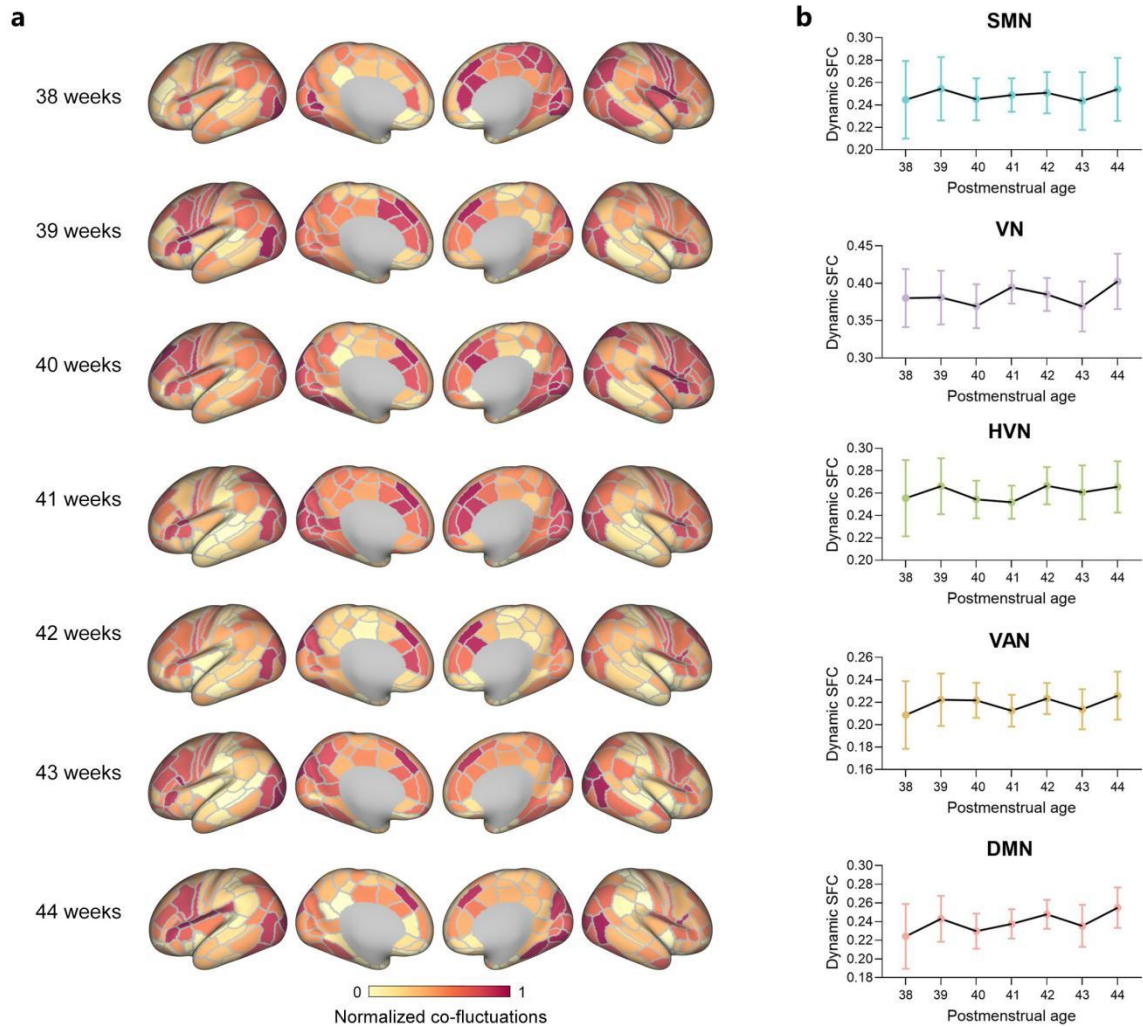
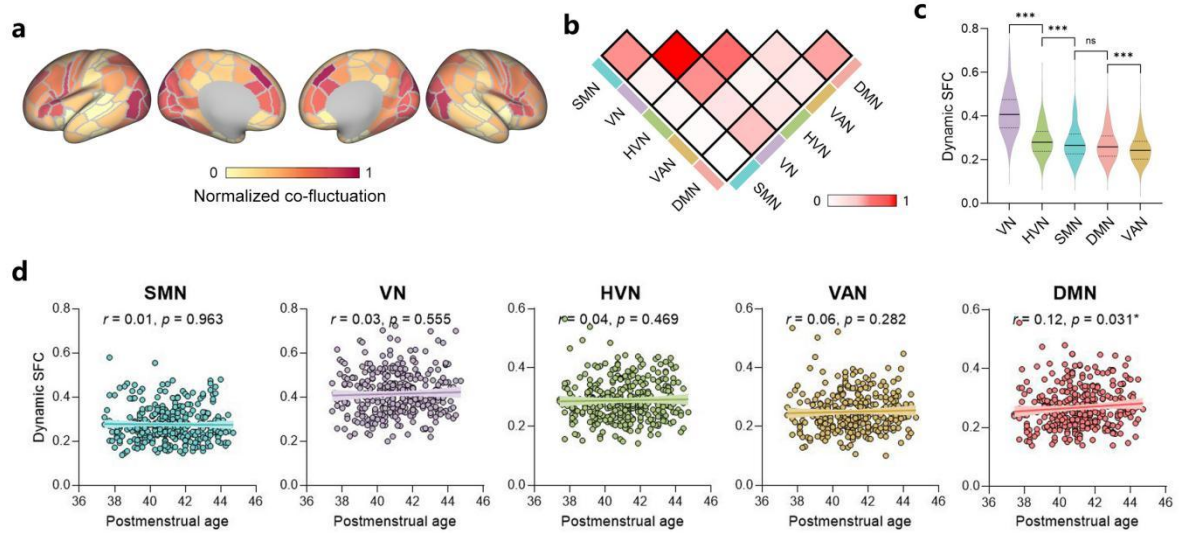


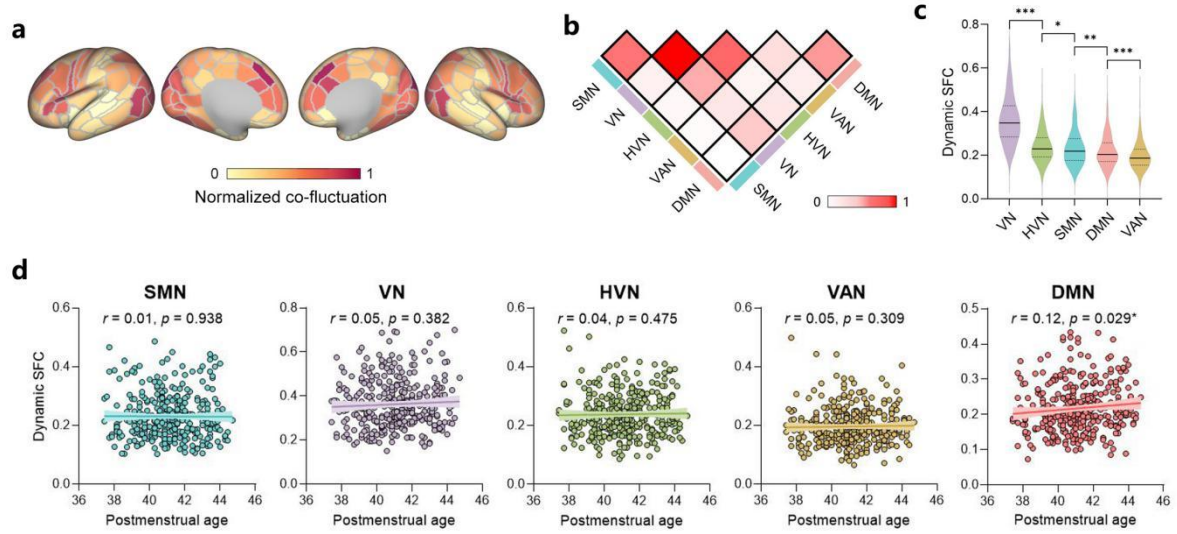
Supplementary material



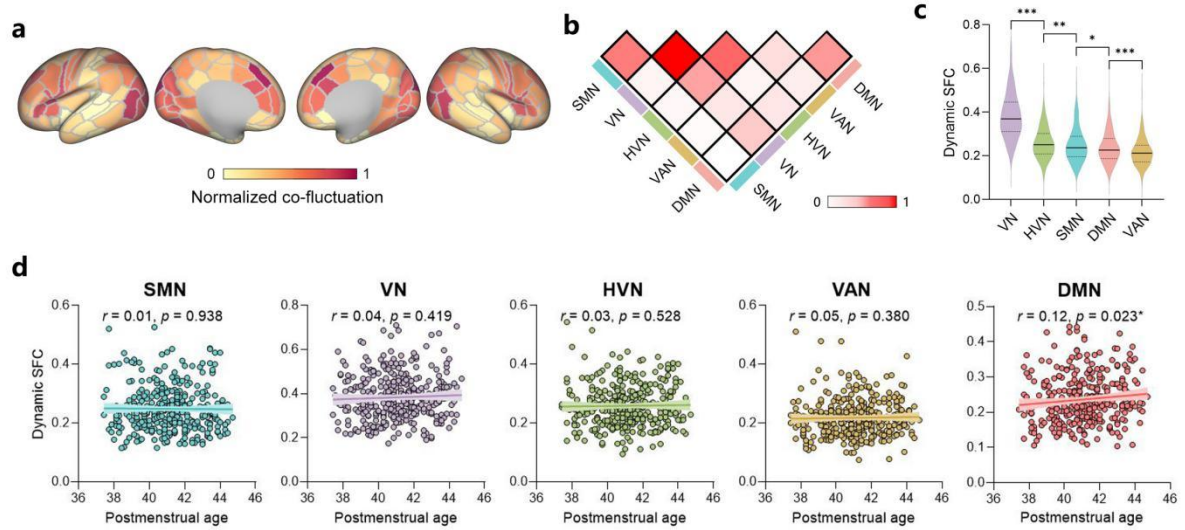
Supplementary Figure 1. The development trajectories of dynamic structure-function coupling (SFC) in term-born infants. (a) Regional dynamic SFC maps across postmenstrual age (PMA). (b) Intra-network dynamic SFC across PMA. SMN, sensorimotor network; VN, visual network; HVN, high-level visual network; VAN, ventral attention network; DMN, default mode network.



Supplementary Figure 2. Dynamic SFC pattern in term-born infants with sliding window size of 80 TRs. (a) Regional dynamic SFC maps, which varies markedly across the neocortex. (b) Subnetwork-level dynamic SFC. (c) Violin plots showing intra-network dynamic SFC of each RSN. (d) Scatter plot showing the relevance between postmenstrual age and intra-network dynamic SFC of the RSNs. A positive association between postmenstrual age and intra-network dynamic SFC was identified within the DMN ($r = .12, P = .031$, FDR-corrected). * $P < .05$, *** $P < .001$.



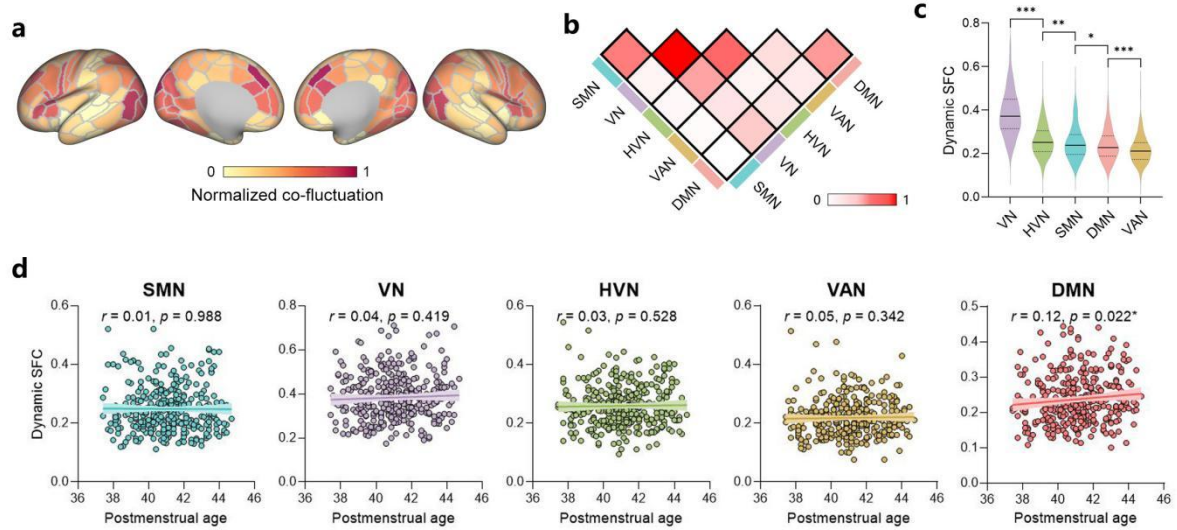
Supplementary Figure 3. Dynamic SFC pattern in term-born infants with sliding window size of 120 TRs. (a) Regional dynamic SFC maps, which varies markedly across the neocortex. (b) Subnetwork-level dynamic SFC. (c) Violin plots showing intra-network dynamic SFC of each RSN. (d) Scatter plot showing the relevance between postmenstrual age and intra-network dynamic SFC of the RSNs. A positive association between postmenstrual age and intra-network dynamic SFC was identified within the DMN ($r = .12, P = .029$, FDR-corrected). * $P < .05$, ** $P < .01$, *** $P < .001$.



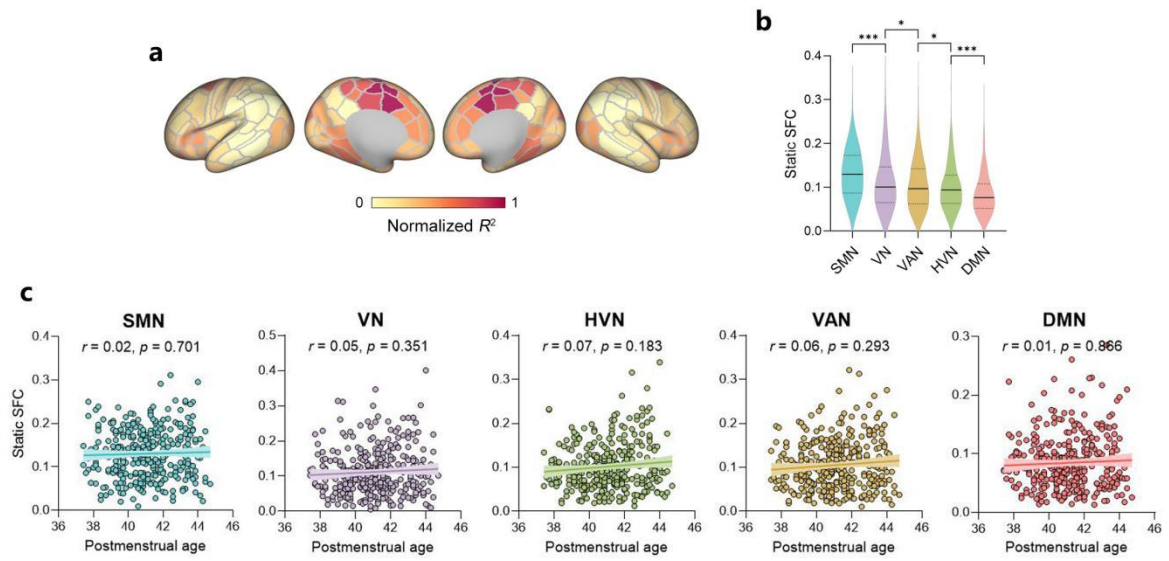
Supplementary Figure 4. Dynamic SFC pattern in term-born infants with steps of 5 TRs.

(a) Regional dynamic SFC maps, which varies markedly across the neocortex. (b) Subnetwork-level dynamic SFC. (c) Violin plots showing intra-network dynamic SFC of each RSN. (d) Scatter plot showing the relevance between postmenstrual age and intra-network dynamic SFC of the RSNs. A positive association between postmenstrual age and intra-network dynamic SFC was identified within the DMN ($r = .12, P = .023$, FDR-corrected).

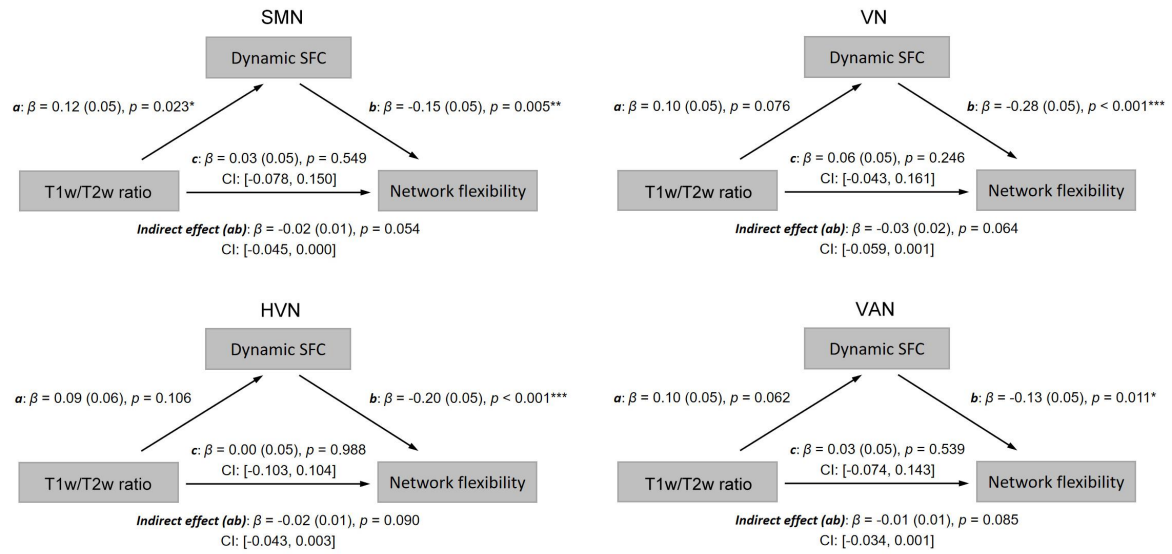
* $P < .05$, ** $P < .01$, *** $P < .001$.



Supplementary Figure 5. Dynamic SFC pattern in term-born infants with steps of 20 TRs. (a) Regional dynamic SFC maps, which varies markedly across the neocortex. (b) Subnetwork-level dynamic SFC. (c) Violin plots showing intra-network dynamic SFC of each RSN. (d) Scatter plot showing the relevance between postmenstrual age and intra-network dynamic SFC of the RSNs. A positive association between postmenstrual age and intra-network dynamic SFC was identified within the DMN ($r = .12$, $P = .022$, FDR-corrected). * $P < .05$, ** $P < .01$, *** $P < .001$.

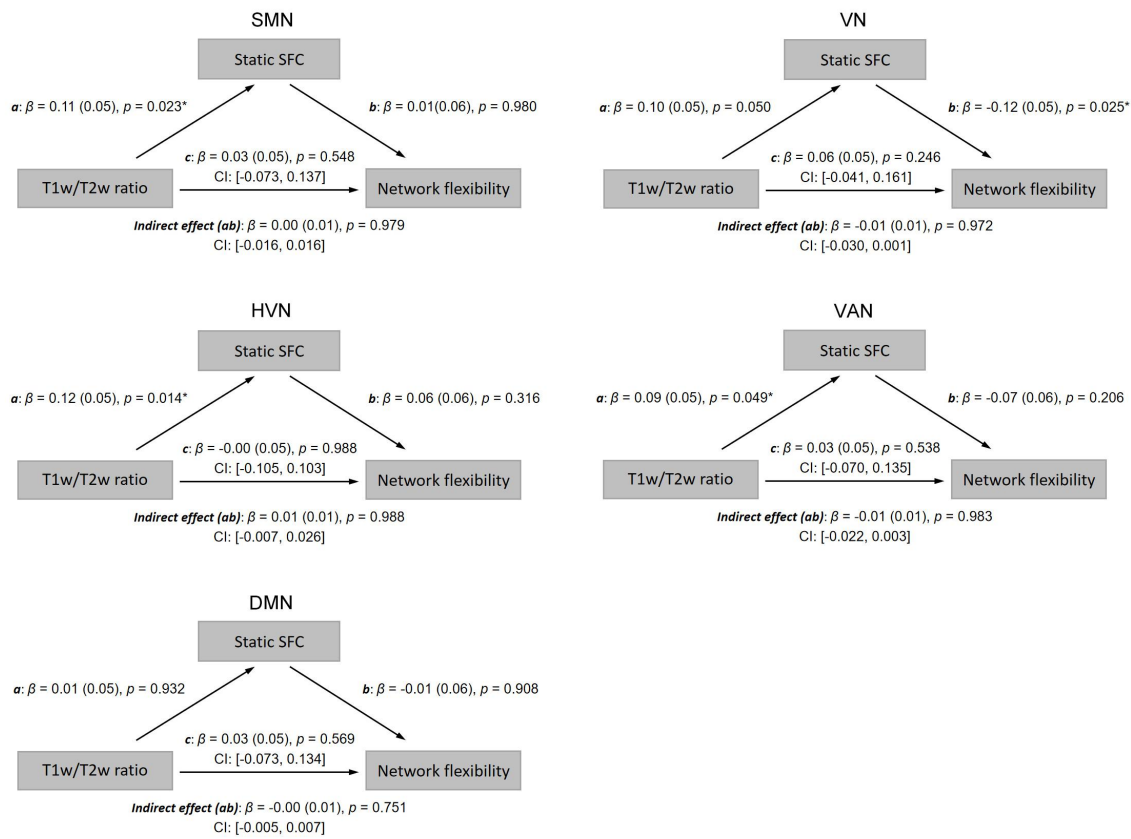


Supplementary Figure 6. Static SFC pattern in term-born infants. (a) Regional static SFC maps, which varies markedly across the neocortex. (b) Violin plots showing intra-network static SFC of each RSN. (c) Scatter plot showing the relevance between postmenstrual age and intra-network static SFC of the RSNs. * $P < .05$, *** $P < .001$.

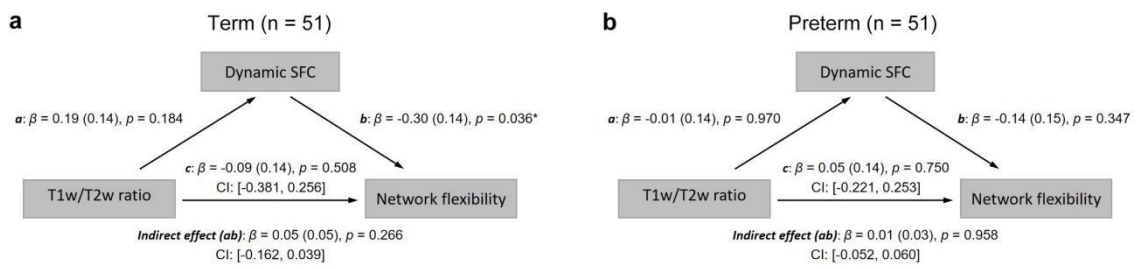


Supplementary Figure 7. Mediation analysis for the other four resting-state networks.

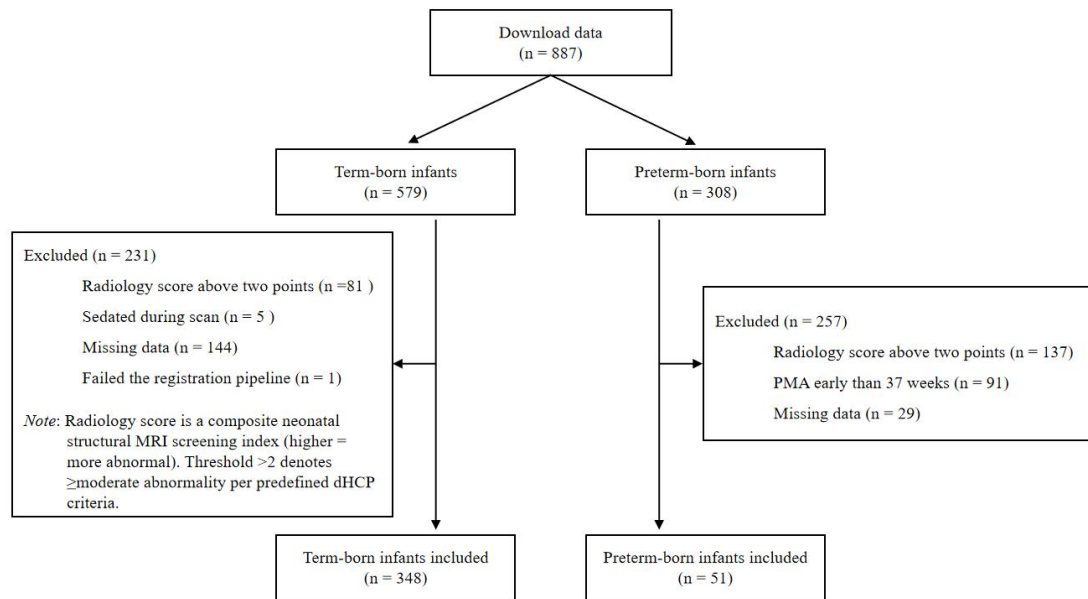
T1w/T2w ratio was set as an independent variant, the network flexibility was a dependent variant, and the dynamic SFC was the mediated variant. Mediation results are presented as standardized regression coefficients, and statistical significance was assessed using 95% bootstrapped confidence intervals. Standard errors are provided in parentheses. $P < .05$, $^{**} P < .01$, $^{***} P < .001$.



Supplementary Figure 8. Mediation analysis using static SFC as the mediator. T1w/T2w ratio was set as an independent variant, the network flexibility was a dependent variant, and the static SFC was the mediated variant. Mediation results are presented as standardized regression coefficients, and statistical significance was assessed using 95% bootstrapped confidence intervals. Standard errors are provided in parentheses. * $P < .05$.

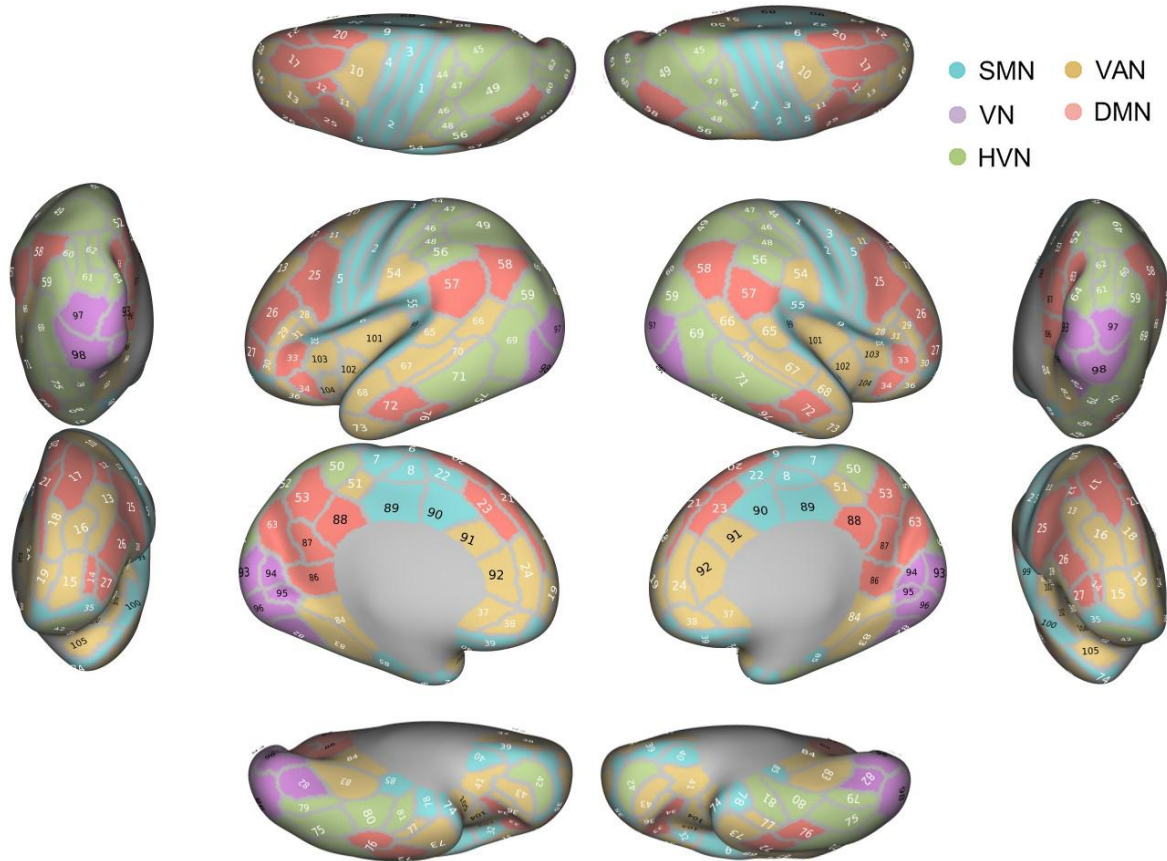


Supplementary Figure 9. Mediation analysis in the default mode network for the subset of term-born infants (a) and the preterm-born infants (b). T1w/T2w ratio was set as an independent variant, the network flexibility was a dependent variant, and the dynamic SFC was the mediated variant. Mediation results are reported as standardized regression coefficients, and statistical significance was assessed using 95% bootstrapped confidence intervals. Standard errors are provided in parentheses. * $P < .05$.

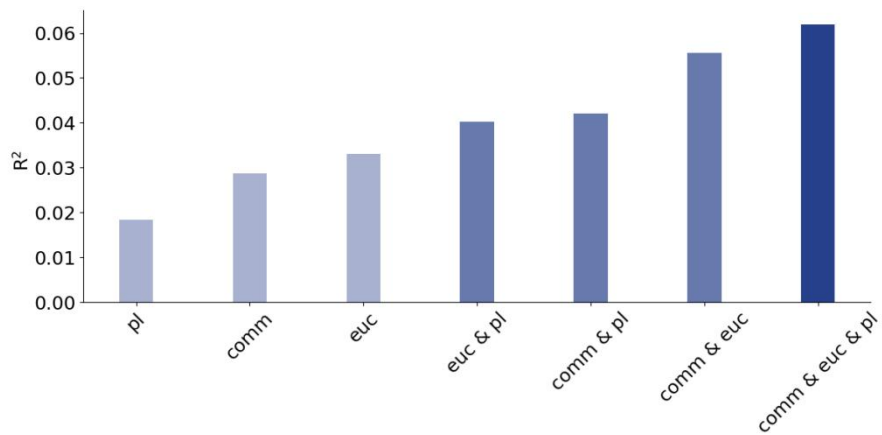


Supplementary Figure 10. Flowchart showing the inclusion of neonates for this study.

PMA refers to age at the time of the MRI scanning. Note that the MRI scans in the dHCP were reviewed by a specialist perinatal neuroradiologist who scored each subject using the following scale: 1. Normal appearance for age; 2. Incidental findings with unlikely significance for clinical outcome or analysis (e.g. subdural haemorrhage. Isolated subependymal cysts. Mild inferior vermis rotation); 3. Incidental findings with unlikely clinical significance but possible analysis significance (e.g. several punctate lesions or other focal white matter / cortical lesions not thought to be of clinical significance); 4. Incidental findings with possible clinical significance. Unlikely analysis significance (e.g. Isolated non brain anomaly for example in pituitary / on tongue); 5. Incidental finding with possible / likely significance for both clinical and imaging analysis (e.g. Major lesions within white matter cortex, cerebellum and or basal ganglia; small head / brain < 1st centile); 6. Q, meaning poor quality anatomical data.



Supplementary Figure 11. Li' 210 multi-modal neonate-specific atlas. SMN, sensorimotor network; VN, visual network; HVN, high-level visual network; VAN, ventral attention network; DMN, default mode network.



Supplementary Figure 12. Explained variance of SFC for single, pairwise, and combined structural predictors. Mean SFC (R^2) across subjects is shown for Euclidean distance (euc), path length (pl), and communicability (comm) modeled alone, in pairs, and combined in a multilinear regression. The monotonic R^2 gain from single to paired to triplet models indicates partially distinct contributions beyond shared variance.