Ideas on molecular dynamics

Wei, R.K.J., Wee, J., Laurent, V.E. *et al.* Hodge theory-based biomolecular data analysis. *Sci Rep* (2022)

- Hodge Laplacian based bimolecular structure analysis

    - Bimolecular topological features: rings, channels, cages, voids…

    - Hodge Laplacian eigenvectors

- Hodge decomposition: to quantify the folding or compactness of molecules

    - To measure the curvedness of the biomolecular chains

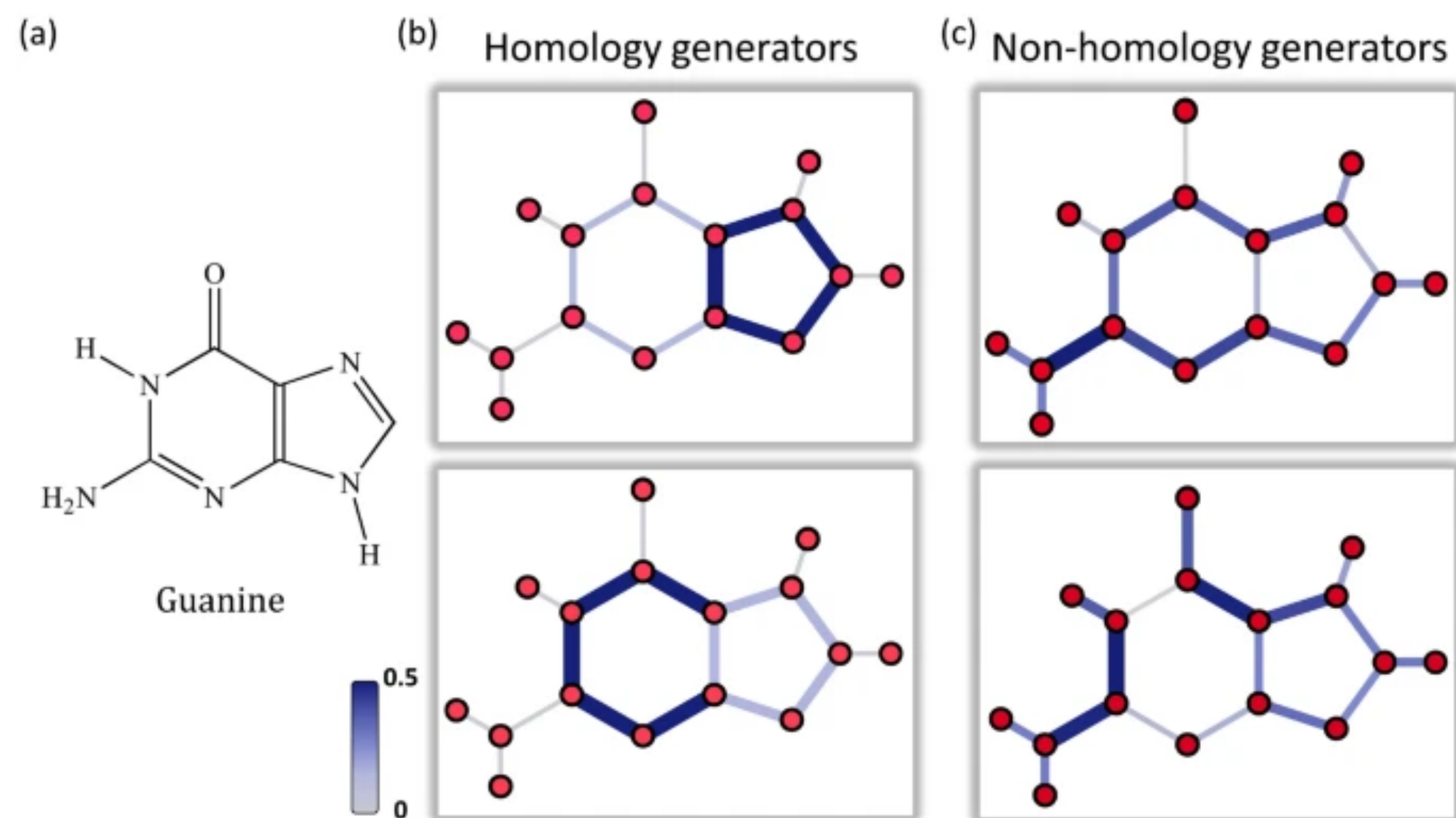   - if i_1, i_2, i_3 are in a straight line, we have zero sum

$$Y_{[i_1,i_2]} = \begin{cases} |\mathbf{r}_{i_1} - \mathbf{r}_{i_2}| & i_1 < i_2, \\ -|\mathbf{r}_{i_1} - \mathbf{r}_{i_2}| & i_1 > i_2. \end{cases}$$

$$Y_{[i_1,i_2]} + Y_{[i_2,i_3]} + Y_{[i_3,i_1]} = 0$$

$$\text{TI} = \sum_{[i,j] \in K} \left| \frac{(Y^c + Y^h)_{[i,j]}}{Y_{[i,j]}} \right|, \qquad \text{AI} = \frac{1}{N} \sum_{[i,j] \in K} \left| \frac{(Y^c + Y^h)_{[i,j]}}{Y_{[i,j]}} \right|,$$

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(a) The graph representation for Guanine. (b) The zero-eigenvalue-related eigenvectors are homology generators. Geometrically, their largest absolute values indicate the associated loop structures. (c) Nonzero-eigenvalue-related eigenvectors are more related to domain, cluster and community structures.
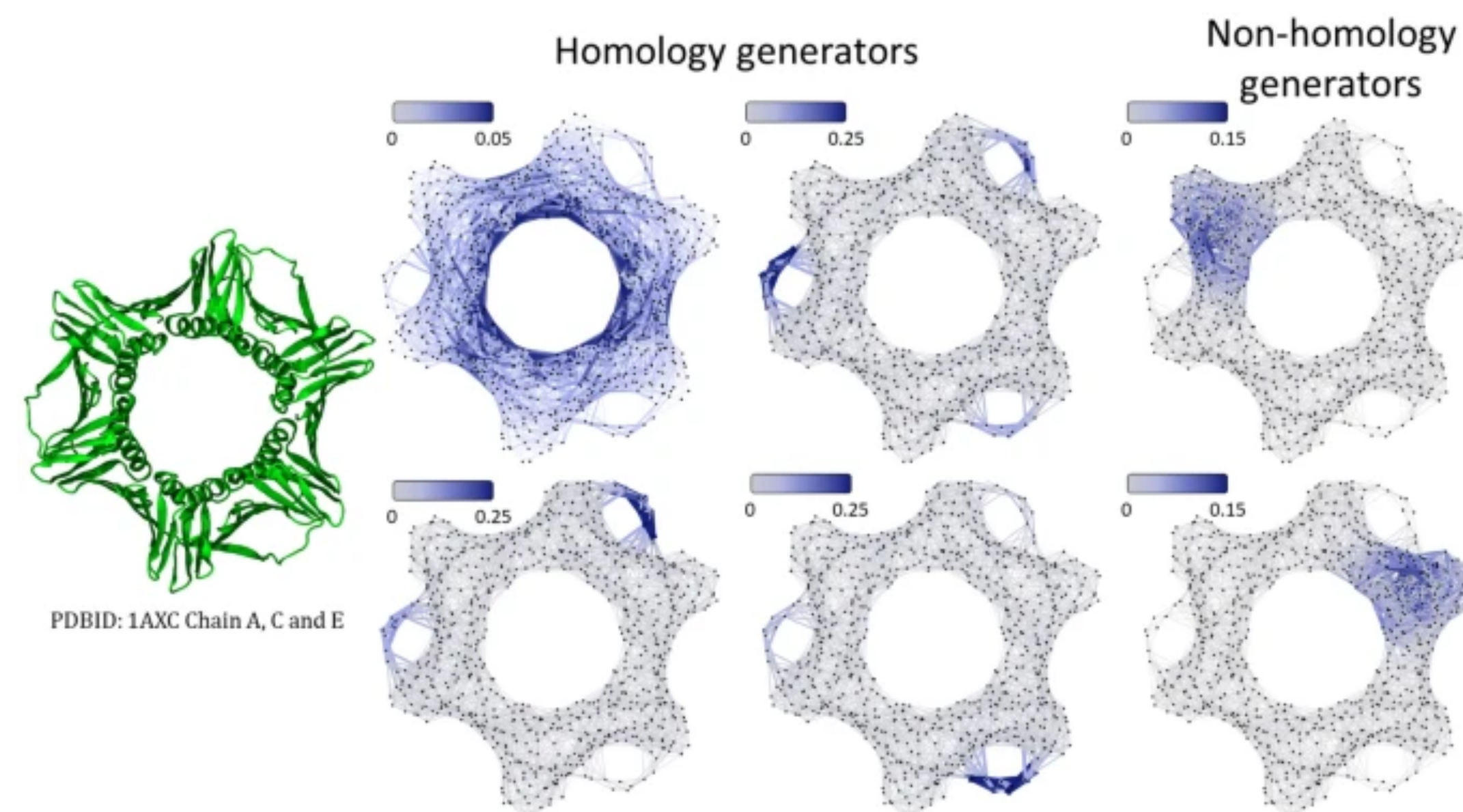
protein structure analysis for protein (ID:1AXC). Four 1D homology generators are from four zero eigenvalue related eigenvectors of 1D HL matrix. Two non homology generators are from two smallest nonzero eigenvalue related eigenvectors. Homology generators characterize loop and cycle structures, while non-homology generators indicate information about domains and communities.