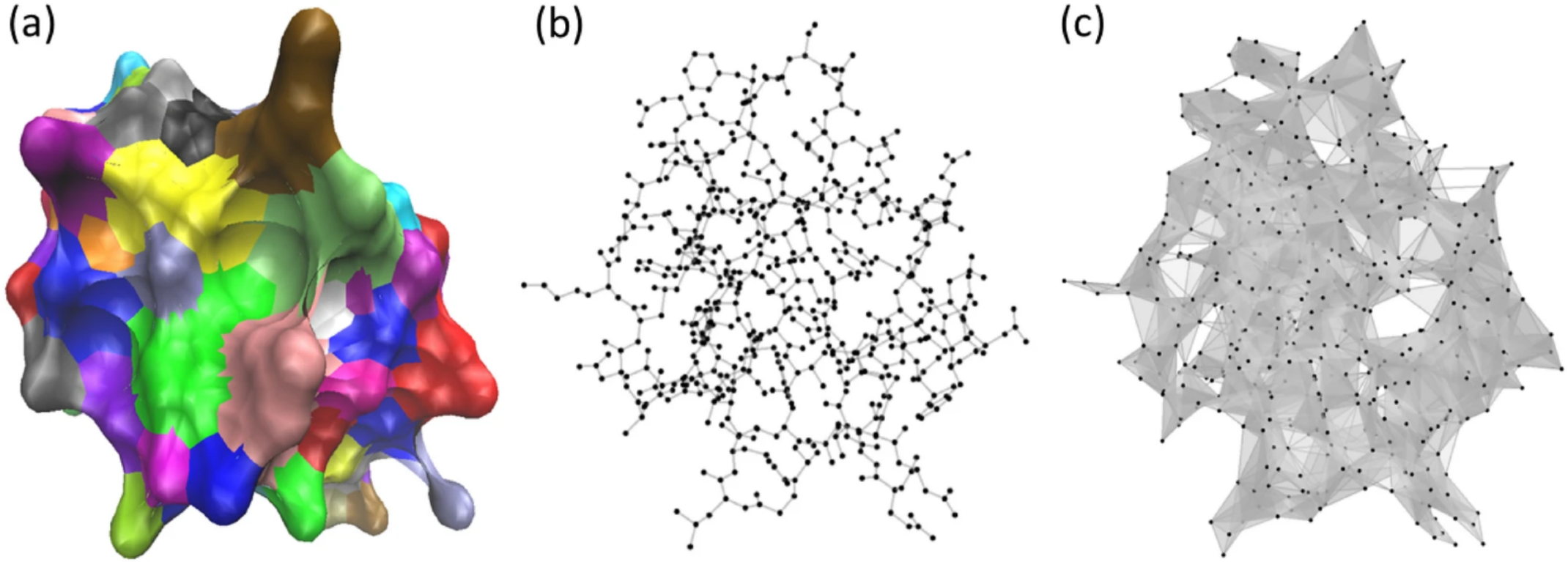
Ideas on molecular dynamics

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



molecular graph and simplicial complex representations for a protein (ID:2OFS)

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- 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

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

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

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