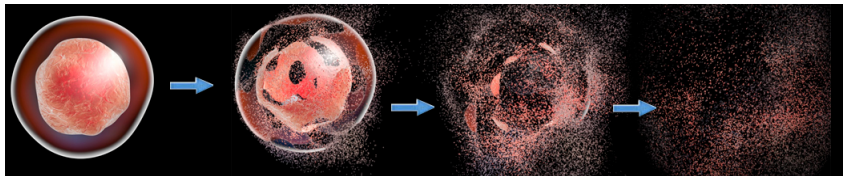


# Computational analysis of bioactive compounds from sugar cane residues

March 16, 2022

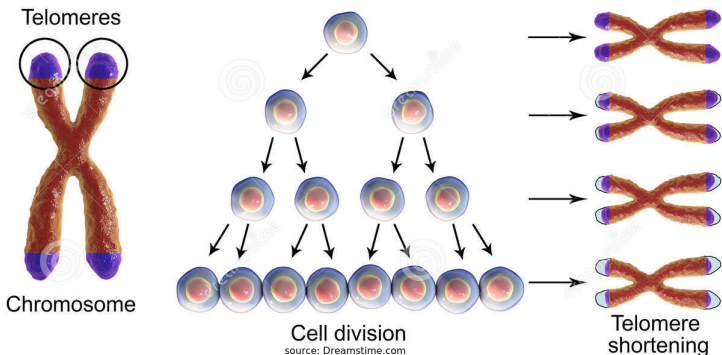
# Apoptosis is programmed cell death



Source: Seamus J. Martin, in *Encyclopedia of Immunology* (Second Edition), 1998

- ▶ Apoptosis is a type of cell death in which a series of molecular steps in a cell lead to its death.
- ▶ This is one method the body uses to get rid of unneeded or abnormal cells.

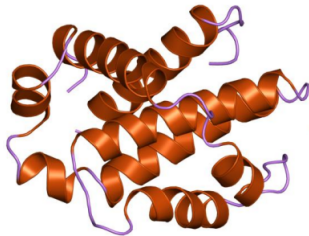
# Apoptosis and aging



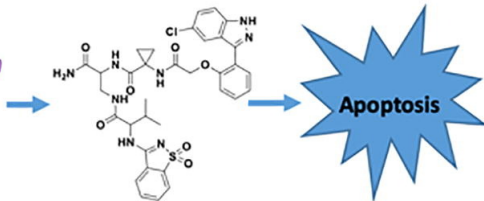
- ▶ Telomeres are specialized structures that cap the ends of eukaryotic chromosomes.
- ▶ Telomere length shortens with each cell replication.
- ▶ This progressive shortening is associated with cellular senescence and apoptosis.

# Regulation of apoptosis

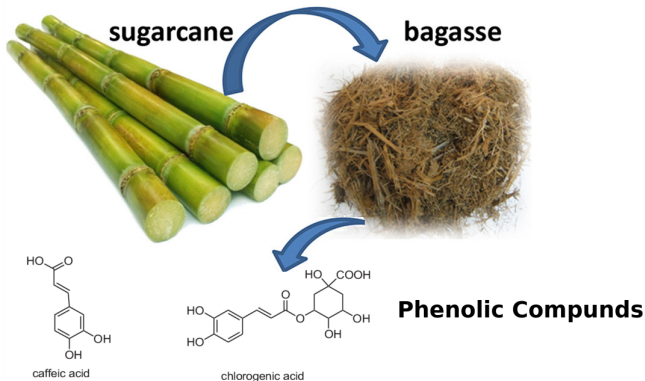
**Target proteins  
(BCL-2 Proteins)**



**Small molecules  
(Phenols)**



# Phenolic compounds from sugarcane bagasse

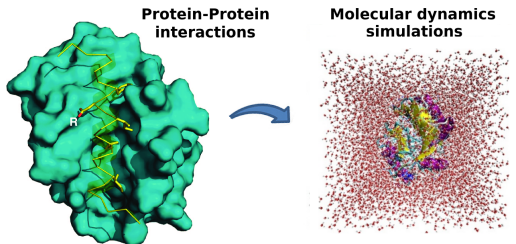


- ▶ An example of these small molecules are the phenolic compounds from agricultural residues like sugarcane bagasse.
- ▶ In Colombia, sugarcane production is the second most important line of agricultural production after coffee<sup>a</sup>.

<sup>a</sup>[https://revistas.uptc.edu.co/index.php/ciencia\\_agricultura/article/view/12823s](https://revistas.uptc.edu.co/index.php/ciencia_agricultura/article/view/12823s)

# Interactions between BCL-2 and phenolic compounds.

- ▶ We will use a computational approach by molecular dynamics.
- ▶ We will study the Protein-protein interactions between BCL-2 and phenolic compounds.



We expect to elucidate the potential mechanisms of antiproliferative action of these phenolic compounds.