1. Draw an analogy of each organelle with (and explain why, in terms of its function):

a. A job in the factory:

Clothing factory	Cell organelle	Function of the organelle
Owner/Chief Operating Officer	Nucleus	Controls all cell activity - similar to the owner or CEO of the factory that oversees all the operations in the factory
Structure of the building (e.g., walls)	Cytoskeleton	Maintains cell shape
Welcome entrance/reception	Cell membrane	Regulates what enters and exits the cell - similar to the entrance of the factory
Factory floor	Cytoplasm	Contains the organelles – similar to the factory floor which is the site of most activity
Energy room	Mitochondria	Powerhouse of the cell - produce energy needed to keep the factory running
Assembly line: cutting, sewing, pressing room	Endoplasmic Reticulum (ER)	Synthesis, folding, modification, and transport of proteins - similar to the assembly line where the production of clothing is completed in a pre-defined sequence (e.g., cutting, sewing, pressing)
Packaging/shipping department	Golgi Apparatus	Proteins received from the ER are further processed and sorted for transport to their final destinations - similar to the packaging/shipping department where they receive items from the assembly line and then pack and distribute them.
Factory workers	Ribosomes	Site of protein production – similar to workers that produce the clothing
Cleaning services	Lysosomes	Breaking down cellular waste – similar to the cleaning services that gets rid of the waste

b. A relevant person or infrastructure in a country

Hospital	Cell organelle	Function of the organelle
Owner/Chief Operating Officer	Nucleus	Controls all cell activity - similar to the owner or CEO of the hospital that makes important decisions for the hospital's welfare
Structure of the building (e.g., walls)	Cytoskeleton	Maintains cell shape
Welcoming entrances/reception (e.g., entrance for out-patient, rehabilitation, emergency)	Cell membrane	Regulates what enters and exits the cell - similar to the entrances of the hospital
Hospital floor	Cytoplasm	Contains the organelles – similar to the hospital floor which is the site of most activity
Electricity/power generator	Mitochondria	Powerhouse of the cell – produce energy needed to keep the hospital running
Nurses	Endoplasmic Reticulum (ER)	Synthesis, folding, modification, and transport of proteins - similar to nurses that takes care of the patients, evaluate their conditions, and accompany/move patients in hospitals
Mail department	Golgi Apparatus	Modifies, sorts, and packages proteins – similar to mail department that sorts, packages, and sends important mail
Doctors	Ribosomes	Site of protein production which is important for the cell – the doctors are important in the hospital, because it is the doctors that give the appropriate treatment so the patients can be healthy
Cleaning services	Lysosomes	Breaks down and gets rid of waste – similar to cleaning services that handles all the waste and disposes them properly

c. Any type of member, fan, or infrastructure of a football club

Football team	Cell organelle	Function of the organelle
Coach	Nucleus	Controls all cell activity - similar to the coach that tells players what to do
Referees	Cytoskeleton	Maintains cell shape – in a way the referees provide a structure for the game (e.g., enforcing the rules)
Sidelines - white or colored lines which mark the outer boundaries of a sports field	Cell membrane	Surrounds the cell and protects it – similar to the sidelines that acts as a barrier between the inside of the field (where the players play), and outside of the field
Playing field	Cytoplasm	Contains the organelles – similar to the playing field where the game is
Sports drink	Mitochondria	Powerhouse of the cell – gives the players the energy needed to play the game
Team's staff/Soccer assistants	Endoplasmic Reticulum (ER)	Synthesis, folding, modification, and transport of proteins – similarly, these assistants prepare, do quality check, and transport the materials needed by the players (e.g., sports drink)
Sports bag	Golgi Apparatus	Modifies, sorts, and packages proteins – similarly, the team's needs are packed in the sports bag
Supporters/Cheerleaders/Family members	Ribosomes	Site of protein production which is important for the cell – similarly, these supporters motivate and encourage players during the game
Cleaning services	Lysosomes	Breaks down and gets rid of waste – cleans the football field

2 pH of ancient waters on Mars : pH $\simeq 3$

a) single E. coli bacteria , $l = 2\ \mu m$

$d = 1\ \mu m$

How many ions may such a bacteria have in Mars ?

- Volume of bacteria $= \pi r^2 L$

$$= \pi (0.5\ \mu m)^2 (2\ \mu m)$$

$$= \pi\ 0.5\ \cancel{\mu m^3} \times \frac{(10^{-5})^3\ \cancel{dm^3}}{1\ \cancel{\mu m^3}} \times \frac{1\ L}{1\ \cancel{dm^3}}$$

$$= \pi (0.5 \times 10^{-15})\ L$$

- $pH = -\log_{10}\left(\frac{[H^+]}{C_0}\right)$

$$3 = -\log_{10}\left(\frac{[H^+]}{C_0}\right)$$

$$[H^+] = 10^{-3}\ C_0 = 10^{-3}\left(\frac{1\ mol}{L}\right)$$

Finally,

$$\frac{\#[H^+]}{\text{bacteria}} = \frac{10^{-3}\ \cancel{mol}}{\cancel{L}} \times \frac{\pi(0.5 \times 10^{-15})\cancel{L}}{\text{bacteria}} \times \frac{6.022 \times 10^{23}\ \text{ions}}{1\ \cancel{mol}}$$

$$\boxed{\approx 9 \times 10^{+5}\ \text{ions for a bacteria in Mars}}$$

Compare this number to that of the same bacteria living on Earth

- Volume of bacteria $= \pi(0.5 \times 10^{-15})\ L$
- $pH = 7$

$$[H^+] = 10^{-7}\ \frac{mol}{L}$$

$$\frac{\#[H^+]}{\text{bacteria on Earth}} = \frac{10^{-7}\ mol}{L} \times \frac{\pi(0.5 \times 10^{-15})\ L}{\text{bacteria on Earth}} \times \frac{6.022 \times 10^{23}\ \text{ions}}{1\ mol}$$

$$\boxed{\approx 90\ \text{ions for a bacteria on Earth}}$$

- The no. of ions for a single E. coli bacteria on Earth is less than that of the same bacteria on Mars

b) For a population of bacteria whose length L is not fixed but follows the distribution

$$P(l) = \frac{1}{\Gamma(k)} \frac{e^{-l/L}}{l} \left(\frac{l}{L}\right)^k$$

i) Check that the length distribution is normalized

$$\int_0^\infty \frac{1}{\Gamma(k)} \frac{e^{-l/L}}{l} \left(\frac{l}{L}\right)^k dl = 1$$

$$\frac{1}{\Gamma(k)} \int_0^\infty \frac{e^{-l/L}}{l} \left(\frac{l}{L}\right)^k dl = 1 \quad ; \quad u = \frac{l}{L} \quad du = \frac{dl}{L}$$

$$l = uL$$

$$\frac{1}{\Gamma(k)} \int_0^\infty \frac{e^{-\cancel{u}}}{u\cancel{L}} (u)^k \cancel{L}\ du = 1$$

$$\frac{1}{\Gamma(k)} \underbrace{\int_0^\infty u^{k-1} e^{-u}\ du}_{} = 1$$

$$\frac{1}{\Gamma(k)} \cdot \Gamma(k) = 1$$

$$1 \stackrel{\checkmark}{=} 1$$

ii) compute its mean and variance :

Mean :

$$\mathbb{E}[\ell] = \int_0^\infty P(\ell)\, \ell \, d\ell$$

$$= \int_0^\infty \frac{1}{\Gamma(k)} \frac{e^{-\ell/L}}{\cancel{\ell}} \left(\frac{\ell}{L}\right)^k \cancel{\ell}\, d\ell$$

$$= \frac{1}{\Gamma(k)} \int_0^\infty e^{-\ell/L} \left(\frac{\ell}{L}\right)^k d\ell \qquad u = \frac{\ell}{L} \quad du = \frac{d\ell}{L}$$

$$= \frac{1}{\Gamma(k)} \int_0^\infty e^{-u} (u)^k \, L\, du$$

$$= \frac{L}{\Gamma(k)} \underbrace{\int_0^\infty e^{-u} u^k \, du}$$

$$= \frac{L}{\Gamma(k)} \cdot \Gamma(k+1)$$

$$= \frac{L\, k!}{(k-1)!} = \frac{(L)\, k\, \cancel{(k-1)!}}{\cancel{(k-1)!}} = Lk$$

$$\boxed{\mathbb{E}[\ell] = Lk}$$

Variance :

$$\mathbb{V}[\ell] = \mathbb{E}[\ell^2] - (\mathbb{E}[\ell])^2$$

$$* \ \mathbb{E}[\ell^2] = \int_0^\infty \frac{1}{\Gamma(k)} \frac{e^{-\ell/L}}{\cancel{\ell}} \left(\frac{\ell}{L}\right)^k \ell^{\cancel{2}}\, d\ell$$

$$= \frac{1}{\Gamma(k)} \int_0^\infty e^{-\ell/L} \left(\frac{\ell}{L}\right)^k \ell \, d\ell \qquad u = \frac{\ell}{L} \quad du = \frac{d\ell}{L}$$

$$\ell = uL$$

$$= \frac{1}{\Gamma(k)} \int_0^\infty e^{-u} (u)^k (uL)(L\, du)$$

$$= \frac{L^2}{\Gamma(k)} \underbrace{\int_0^\infty u^{k+1} e^{-u} du}$$

$$= \frac{L^2}{\Gamma(k)} \cdot \Gamma(k+2) = \frac{L^2 (k+1)!}{(k-1)!} = \frac{L^2 (k+1)(k)\cancel{(k-1)!}}{\cancel{(k-1)!}}$$

$$= L^2(k^2+k)$$

$$\mathbb{V}(\ell) = \mathbb{E}[\ell^2] - (\mathbb{E}[\ell])^2$$

$$= L^2(k^2+k) - L^2k^2$$

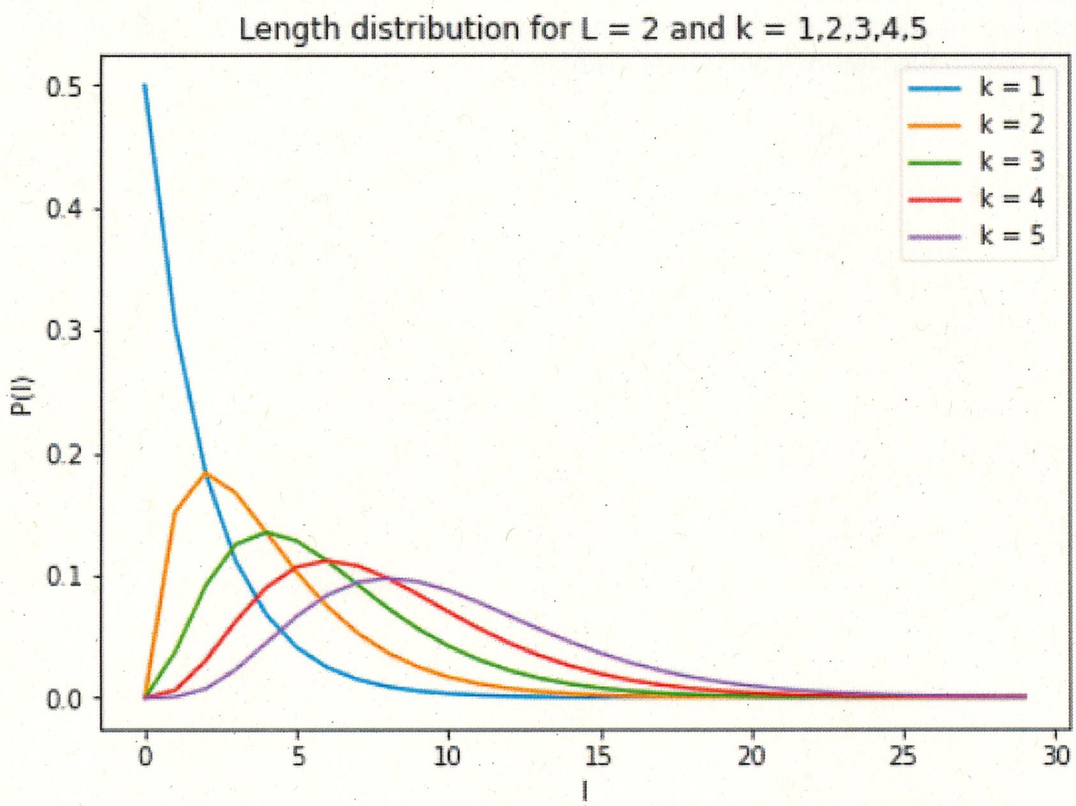
$$\boxed{\mathbb{V}(\ell) = L^2 k}$$

```
[1]: import numpy as np
     import scipy.special as sp
     import matplotlib.pyplot as plt
```

iii) Plot the length distribution for L = 2 and k = 1, 2, 3, 4, 5

```
[2]: L = 2
     final_list = []
     #iterate over different values of k
     for k in [1,2,3,4,5]:
         y_list = []
         #iterate over different values of l
         for l in range(0,30):
             y = (1 / sp.gamma(k)) * ( np.exp(-l/L) / L ) * ( (l/L)**(k-1) )
             y_list.append(y)
         final_list.append(y_list)
```

```
[3]: #plot figure
     plt.figure(figsize=(7,5))
     labels = ['k = 1', 'k = 2', 'k = 3', 'k = 4', 'k = 5']
     for i,j in zip(final_list, labels):
         plt.plot(i, label = j)
         plt.legend()
     plt.xlabel('l')
     plt.ylabel('P(l)')
     plt.title('Length distribution for L = 2 and k = 1,2,3,4,5')
     plt.show()
```



iv) What is the distribution $P(V)$ of the volume of the bacteria?

$$V = A \cdot \ell$$
$$= \frac{\pi d^2}{4} \cdot \ell \quad \rightarrow \quad \ell = \frac{4V}{\pi d^2}$$

$$P(\ell) = \frac{1}{\Gamma(k)} \frac{e^{-\ell/L}}{\ell} \left(\frac{\ell}{L}\right)^k$$

$$P(V) = A \cdot P(\ell)$$
$$P(V) = \frac{\pi d^2}{4} \cdot \frac{1}{\Gamma(k)} \frac{\pi d^2}{4V} e^{-\left(\frac{4V}{\pi d^2 L}\right)} \left(\frac{4V}{\pi d^2 L}\right)^k$$

(3) Information bits on the human genome

a) What's the length of human's genome (in basepairs)?

$$\boxed{\text{total basepairs} = 3 \times 10^{9}\ \frac{\text{basepairs}}{\text{individual}}}$$

What would be its length in kilometers?

$$3.4 \times 10^{-10}\ \frac{\cancel{m}}{\cancel{\text{basepairs}}} \times 3 \times 10^{9}\ \frac{\cancel{\text{basepairs}}}{\text{individual}} \times \frac{1\ \text{km}}{1{,}000\ \cancel{m}} = \boxed{1.02 \times 10^{-3}\ \text{km}}$$

Bionumbers source: Watson JD, Crick FH. Molecular structure of nucleic acids a structure for deoxyribose nucleic acid. Nature. 1953 Apr 25 171(4356): 737-8. p. 737

b) Consider a minimal polymerization model of single-stranded DNA in w/c each basepair (A, C, G, T) is added to the template w/ equal probability following an i.i.d process. What is the total (Shannon) entropy, in bits of the entire human genome

$$H(x) = \sum_{i=1}^{|x|} P_i \log_2 \frac{1}{P_i}$$

A with prob. 1/4
C with prob. 1/4
G with prob. 1/4
T with prob. 1/4

Total Shannon entropy:

$$H(x) = \frac{1}{4}\log_2 4 + \frac{1}{4}\log_2 4 + \frac{1}{4}\log_2 4 + \frac{1}{4}\log_2 4$$

$$= 2$$

Total Shannon entropy of the entire human genome $= 2 \times 3 \times 10^{9}$ basepairs

$$= \boxed{6 \times 10^{9}}$$

4 Assume that a cell is a spherical capacitor

thickness $\delta = 4nm = 4 \times 10^{-9}$ m

outer shell radius $R = 5\ \mu m = 5 \times 10^{-6}$ m

transmembrane potential $\phi = 60$ meV

relative permitivity $\varepsilon_r = 2$

a) What is the value of Q in Coulombs?

$$Q = \frac{4\pi \varepsilon_0 \varepsilon_r}{\left(\frac{1}{R-\delta} - \frac{1}{R}\right)} V = \frac{4\pi \varepsilon_0 \varepsilon_r}{\left(\frac{\delta}{R(R-\delta)}\right)} V = \frac{4\pi \varepsilon_0 \varepsilon_r \cdot R(R-\delta) V}{\delta} =$$

$$= \frac{4\pi \left(8.8 \times 10^{-12} \frac{C}{\cancel{m}\cancel{V}}\right)(2)\left(5 \times 10^{-6} \cancel{m}\right)\left(5 \times 10^{-6} - 4 \times 10^{-9}\right)\cancel{m}\left(60 \times 10^{-3} \cancel{V}\right)}{4 \times 10^{-9} \cancel{m}}$$

$$\boxed{Q \approx 8 \times 10^{-14}\ C}$$

How many protons does it correspond to?

$Q = N_p e$

$$N_p = \frac{Q}{e} = \frac{8 \times 10^{-14} \cancel{C} \times \frac{1\ \cancel{e}}{1.6 \times 10^{-19} \cancel{C}}}{\cancel{e}} = \boxed{5 \times 10^{5} \text{ no. of protons}}$$

b) How much energy does the pump need to transport 1 electron?

Express this result in:

i) eV : 60×10^{-3} eV

ii) J : $60 \times 10^{-3}\ eV \times \frac{1.6 \times 10^{-19}\ J}{1\ eV} = \underline{9.6 \times 10^{-21}\ J}$

iii) K_BT : $9.6 \times 10^{-21}\ J \times \frac{1\ K_BT}{4 \times 10^{-21}\ J} = \underline{2.4\ K_BT}$

How much power does the pump need to develop in order to achieve a current of 1 pA?

i) Watts : $P = VI$

$= 60 \times 10^{-3}\ V\ (1 \times 10^{-12}\ A)$

$= \underline{60 \times 10^{-15}\ W}$

ii) K_BT/s : $60 \times 10^{-15} \frac{\cancel{J}}{s} \times \frac{1\ K_BT}{4 \times 10^{-21} \cancel{J}} = \underline{15 \times 10^{6}\ K_BT/s}$

iii) ATP/s : $15 \times 10^{6} \frac{K_BT}{s} \times \frac{1\ ATP}{14\ K_BT} = \underline{1.1 \times 10^{6}\ ATP/s}$

(from lecture notes)

5. Blood glucose levels should be in the range between 80 and 170 mg of glucose / dL of blood

a) 80 mg / dL to mmol / L → $80 \frac{mg}{dL} \times \frac{10\ dL}{1\ L} \times \frac{1\ mol}{180\ g_{glucose}} = \boxed{4.4\ mmol / L}$

170 mg / dL to mmol / L → $170 \frac{mg}{dL} \times \frac{10\ dL}{1\ L} \times \frac{1\ mol}{180\ g_{glucose}} = \boxed{9.4\ mmol / L}$

How would you transform the time series from mg / dL to mmol / L

$$1 \frac{mg}{dL} \times \frac{10\ dL}{1\ L} \times \frac{1\ mol}{180\ g_{glucose}} = \frac{1}{18} \frac{mmol}{L}$$

$$\boxed{1 \frac{mg}{dL} = \frac{1}{18} \frac{mmol}{L}}$$

b) Estimate how many grams of glucose, weight = 70 kg
glucose level = 125 mg / dL

grams of glucose = $125 \frac{mg}{dL} \times$ volume of blood for a person that weighs 70 kg

↳ % of blood in a human ~8%

For a 70 kg individual, volume of blood is:

$$V = \frac{m}{\rho} = \frac{70\ kg \times 0.08}{1\ g / mL}$$

thus,

$$\text{grams of glucose} = 125 \frac{mg}{\cancel{dL}} \times \frac{10\ \cancel{dL}}{1\ \cancel{L}} \times \frac{70\,000\ \cancel{g} \times 0.08}{1\ \cancel{g} / \cancel{mL}} \times \frac{1\ \cancel{L}}{1{,}000\ \cancel{mL}}$$

$$= 7000\ \cancel{mg} \times \frac{1\ g}{1{,}000\ \cancel{mg}}$$

$$= \boxed{7\ g}$$

Repeat the calculation for a spherical droplet of blood (radius = 1 mm)

grams of glucose = $125 \frac{mg}{dL} \times$ vol. of spherical droplet

↳ $V = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi (1 \times 10^{-3} m)^3$

$$= 125 \frac{mg}{\cancel{dL}} \times \frac{10\ \cancel{dL}}{1\ \cancel{L}} \times \frac{4 \cdot \pi \cdot 1 \times 10^{-9}\ \cancel{m^3}}{3} \times \frac{1{,}000\ \cancel{L}}{1\ \cancel{m^3}}$$

$$= 5 \times 10^{-3}\ mg \times \frac{1\ g}{1{,}000\ mg}$$

$$= \boxed{5 \times 10^{-6}\ g}$$

c) Hypoglycemia happens when blood glucose levels fall below 70 mg/dL
Estimate how many grams in glucose were consumed in the blood system of a patient initially in normal levels (125 mg/dL) that suffers a hypo event

$125\ mg/dL - 70\ mg/dL \rightarrow 55\ \frac{mg}{dL} \times \frac{10\ dL}{1L} \times \frac{70000\ g \times 0.08}{1g\ /mL} \times \frac{1\ L}{1{,}000\ mL}$

$= 55\ mg/dL$

gram in glucose $= 3080\ mg \times \frac{1\ g}{1000\ mg} = \boxed{3.1\ g}$

d) How much energy is consumed by the organism when catabolizing the amount of glucose in the hypo event (c)?

energy (in ATP) $= 3.1\ g \times \frac{1\ mol}{180\ g\ glucose} \times \frac{6.02 \times 10^{23}\ molecules}{1\ mol} \times \frac{30\ ATP}{1\ molecule}$

$= \boxed{3.1 \times 10^{23}\ ATP}$

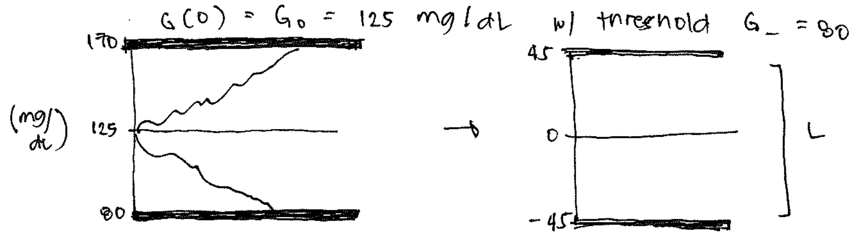
* Bionumbers source : Rich, PR. The molecular machinery of Keilin's respiratory chain. Biochem Soc Trans. 2003 Dec 31 (PT 6) 1095-105 p. 1103

If this event takes 30 min to happen, estimate average power used in the process

$P = \frac{E}{t} = \frac{3.1 \times 10^{23}\ ATP}{30\ mins} = \boxed{1.0 \times 10^{22}\ ATP/mins}$

e) You develop a stochastic model for the evolution of blood glucose levels G(t) as a function of time t

$G(0) = G_0 = 125\ mg/dL$ w/ threshold $G_- = 80\ mg/dL$ and $G_+ = 170\ mg/dL$



What is the value of D_G if the average time for the patient to fall below G_- or pass above G_+ is $\langle \tau \rangle = 2h$?

$\langle \tau \rangle = \frac{(L/2)^2}{6 D_G}$

$D_G = \frac{(45\ mg/dL)^2}{6 \cdot 2\ hrs}$

$= \boxed{168.8\ \frac{mg^2/dL^2}{hrs}}$

6. **Write a 10-sentence summary about one research topic in the talk "Computational Methods in the Discovery of Bioactive Natural Products" https://youtu.be/LMUqQSnvFTA. For this purpose, pick a relevant research article of those included within the references of the seminar.**

The research article that I picked is:

Dietary Antioxidants and Parkinson's Disease (Park, H., & Ellis, A. (2020). Dietary Antioxidants and Parkinson's Disease. Antioxidants, 9(7), 570. doi: 10.3390/antiox9070570)

Parkinson's disease is a neurodegenerative brain disorder caused by the loss of dopaminergic neurons in the basal ganglia. As a result, patients with Parkinson's disease have inadequate levels of dopamine. Since dopamine is responsible for movement-related (motor) system, patients with Parkinson's disease experience motor symptoms such as tremor, and speech difficulties. However, patients also experience nonmotor symptoms such as depression, and insomnia.

Development and progression of this disease is associated with the accumulation of oxidative stress, generated by several factors such as age, lifestyle, and pre-existing conditions. This oxidative stress leads to mitochondrial dysfunction, hindering the energy-demanding process in the brain which leads to symptoms of Parkinson's disease.

Currently there is no treatment to stop the progression of Parkinson's disease, however, lifestyle changes like dietary modification with antioxidants-rich foods can slow the progression of the disease. These dietary antioxidants include vitamin C, vitamin E, carotenoids, selenium, and polyphenols. These antioxidants have neuroprotective roles, including: (1) protecting downstream targets of oxidative stress to alleviate the damage that promotes the development of the disease, and (2) regulating genes that control the growth, and survival of dopaminergic neurons. However, clinical trials are needed to determine whether these antioxidants may act individually or in synergy as a therapeutic intervention of the disease.