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# The effect of Egyptian leek seeds and leaves on colon and breast cancer based on their antioxidant activity and DFT Approach

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## ABSTRACT

Egyptian Leek (*Allium ampeloprasum* var. kurrat) has beneficial effects on human health and possess exceptional nutritional characteristics where they have strong antioxidant properties and inhibit the growth of malignancies. The current study aims to investigate the antioxidant activity and anticancer effect of phytochemical including phenolic compounds, flavonoids, tannins, and alkaloids in leek (seeds and leaves). The current results indicated that the leek leaves are good sources of ash (17.10±1.52 g/100g) and crude fibers (22.40±2.36 g/100g). While leek seeds are good source of protein (25.40±1.62 g/100g) and crude fat (11.37±2.21 g/100g). Leek leaves have high level of polyphenols (0.21±0.075 g/100g), flavonoids (0.57± 0.12 g/100g), alkaloids (0.67±0.018 g/100g) and tannins (556.90 ±0.52 mg tannic acid equivalent /100g). The phytochemicals values are higher in leek leaves than seeds. Linoleic acid (omega-6) is high in leek seeds (57.84 ±0.011 g/100g). Myricetin and Kaempferol are the most abundant flavonoids in leek seeds, while catechol and benzoic acid are the highest non-flavonoids in leek leaves. The obtained results revealed that leek leaves have higher total antioxidant capacity than leek seeds. Leek showed a high anticancer effect on breast cancer cells (MCF-7) and colon cancer cells ($HCT_{116}$) according to the $IC_{50}$ breast cancer cells in the form of the (MCF-7) cell line. Density function theory (DFT) showed that Pyrogallol, Catechol, and Caffeic acid have more powerful antioxidants than the other phenolic compounds.

***Key words*:** Phytochemicals, antioxidant, tannins, phenolic compounds, flavonoids, leek.

## INTRODUCTION

Various physiological activities in human bodies, such as respiration, food digestion, alcohol and drug metabolism, and fat conversion into energy, generate detrimental substances known as free radicals (Jelic *et al*., 2021) which also known as reactive oxygen species (ROS), are highly reactive molecules that continuously circulate throughout the body and are produced as a byproduct of several biochemical events occurring in the human body. The body eliminates them by antioxidant mechanisms such as scavenging free radicals, chelating metals, and employing enzymes to neutralize these reactive substances immediately after their formation. Disruption of these natural mechanisms leads to an excessive accumulation of radicals, which plays a role in the pathogenesis of various diseases such as alzheimer's, parkinson's, diabetes, rheumatoid arthritis, and cancer (Chaudhary *et al*., 2023). Oxidative stress is a crucial factor in the development of chronic diseases such as cardiovascular diseases, diabetes,

neurological disorders, and cancer (Sharifi-Rad *et al.,* 2020). Oxidative stress refers to an imbalance between the generation of ROS and the effectiveness of antioxidants. These correlations highlight the need to achieve a harmonious equilibrium between the plentiful presence of ROS and antioxidants (Jelic *et al*., 2021).

Antioxidants are chemicals that can inhibit or postpone the oxidation process of proteins, lipids, carbohydrates, and DNA in biological systems. They also known as free radical scavengers, function as a protective system that safeguards biomolecules and organisms from the detrimental impact of free radicals. According to Kıran *et al*. (2023), antioxidants have the potential to enhance the immune system's ability to defend against diseases and reduce the likelihood of developing cancer. Antioxidants can be found in both enzymatic or endogenous forms, such as catalase (CAT) and glutathione peroxidase (GPx), as well as non-enzymatic or exogenous forms, such as phytochemicals. These antioxidants are present in both the intracellular and extracellular environment. The body requires both enzymatic and non-enzymatic antioxidants for optimal functioning (Zewen *et al.,* 2018). Phytochemicals are bioactive compounds derived from plants, such as carotenoids, polyphenols, isoprenoids, phytosterols, saponins, dietary fibers, and certain polysaccharides. They exhibit various biological effects, including anti-inflammatory, antimicrobial, and antioxidant activities, which serve to protect plants. The variation in antioxidant properties seen in fruits and vegetables can be due to their diverse components, including ascorbic acid, vitamin E, carotenoids, lycopene, polyphenols, and other phytochemicals (Kumar *et al.,* 2023). Over a thousand phytochemicals exist can be obtained from a variety of sources including whole grains, fruits, vegetables, nuts, and herbs. Polyphenols, including flavonoids and non-flavonoids, are the predominant phytochemicals that exhibit antibacterial, antioxidant, anticancer, anti-inflammatory, and wound-healing properties (Rudrapal *et al*., 2022).

The Egyptian leek (*Allium ampeloprasum* var. kurrat) contain a diverse range of bioactive components such as flavonoids, sulphuric compounds, and saponins (Abd El-Rehem and Ali, 2013) which exhibit different biological activities, including antimicrobial, antihypertensive, antihyperlipidemic, antidiabetic, anti-atherosclerotic, and anticarcinogenic effects (Shahrajabian *et al*., 2021). Leeks (*Allium ampeloprasum* L.) possess exceptional nutritional characteristics and serve as a bountiful reservoir of bioactive substances and phytochemicals and include high levels of dietary fibers, fructans, polyunsaturated fatty acids, diverse amino acids, organic acids, and saponins, which contribute to a range of health advantages (Asemani *et al.,* 2019).

Leek consumption has been found to lower the risk of hypercholesterolemia (Ghasemiyanpour *et al*., 2017), as well as reduce blood pressure, arteriosclerosis, and platelet aggregation. These effects contribute to the prevention of cardiovascular illnesses. In addition, leeks possess antibacterial properties that can effectively combat a wide range of bacteria, fungi, and viruses (Rafiq *et al.,* 2020; Gavanji *et al.,* 2023).

Cancer is a pathological condition due to alterations in DNA (Hazrulrizawati and Normaiza, 2019). Due to the high costs of current chemotherapies, associated side effects, and inefficient treatment regimens, the search for alternative cancer prevention and treatment strategies has become necessary.

Leek seeds and leaves have been utilized in traditional medicine and have demonstrated potential anticancer effects in

several cancer cell lines, such as lung and breast tumors (Hazrulri zawati and Normaiza, 2019; Jia *et al*., 2022). Leek has a diverse range of bioactive components such as flavonoids and sulphuric compounds that have been found to inhibit the growth of malignancies, particularly those affecting the gastrointestinal tract (Shahrajabian *et al*., 2021). Leeks contain allyl sulfides, which have been demonstrated to alter certain pathways related to the proliferation of cancerous tumors (Sergio *et al.,* 2015).

The knowledge of antioxidants in cancer-curing or preventing methods is still in the early stages. The relationship between antioxidants and cancer prevention cannot be depicted only based on the presumed mechanism of action when used. There is sufficient evidence to recommend consuming food sources rich in antioxidants.

This study aims to investigate and assay identify the photochemicals and antioxidant activity and anti-cancer effect of leek (seeds and leaves).

## MATERIALS AND METHODS

### - Materials

**Plants:**

Samples of leek (*Allium porrum* L.) seeds and leaves were purchased from a local market, in El-Fayoum governorate, Egypt, in October 2020.

**Chemicals:**

-Ethanol, methanol and sodium hydroxide (NaOH) were obtained from Al-Gomhouria Company for Trading Chemicals and Instruments, Egypt. 1,1-diphenyl-2-picrylhydrazyl (DPPH) and Aluminum chloride (AlCl3) were obtained from Sigma-Aldrich Company (Saint Louis, MO, USA).

- Human cell lines colon and cell lines human breast ($HCT_{116}$ and MCF7 respectively) were prepared in the National Cancer Institute, Cairo, Egypt.

### - Methods:

**Preparation of Leek leaves powder:**

Egyptian leek (seeds and leaves) were collected fresh without any physical defect; then the samples of leek leaves were sliced into chips and dried in an oven with leek seeds at a temperature of 40°C for 72 hours. After drying, the samples were ground into fine powder by using a commercial blender and passed through a 150µm mesh sieve. The powdered sample was stored in an air-tight bottle and freeze (about -14°C) until analysis (Kashef *et al.,* 2018).

**Chemical analyses of Leek (seeds and leaves):**

The technique provided by A.O.A.C. (2000) was used to determine the chemical components of leek (seeds and leaves) including moisture, crude fiber, protein, total fats, and ash concentrations. The total carbohydrates were calculated by difference.

**Determination of phytochemicals in leek (seeds and leaves):**

- **Determination of total phenols of leek (seeds and leaves):**

The total phenols content in the ethanol extract of leek (seeds and leaves) were measured using the Folin-Ciocalteu's and according to the procedure outlined by Amarowicz *et al.* (2004). The absorbance was measured at 765 nm by spectrophotometer (UV-Vis Jenway 6405, UK). A calibration curve (R2= 9995) of gallic acid (0-0.10 mg/ ml) was prepared and tested under similar conditions. The total phenols were measured using the gallic acid equivalence (GAE) technique.

- **Determination of total flavonoids of leek (seeds and leaves):**

The total flavonoids were measured using the procedure outlined by Fattorusso *et al*., (2002). They were assayed by combining 5 ml of ethanol extract with 3 ml of sodium chloride (2.4%) and 9.8% potassium acetate.

UV-visible spectrophotometer (UV-Vis Jenway 6405, UK) was used to detect the absorbance of the reaction mixture at 420 nm.

- **Determination of fatty acids in leek seeds:**

The production of fatty acid methyl esters (FAME) involves a reaction of methanol and lipids that is catalyzed by an alkali. The process takes place in the presence of 2M potassium hydroxide and is injected into hexane. An Agilent Technologies gas chromatography GC 7890B with flame ionization capabilities was used. A detector was a Zebron ZB-FAME column measuring 60 m x 0.25 mm internal diameter and 0.25 µm film thickness were used to accomplish separation (Kajiwara *et al.,* 2009).

- **Determination of Total alkaloid content (TAC) of leek (seeds and leaves):**

This was measured using Gan *et al*. (2010) method that examine a Thermo Varioskan Flash (Thermo Fisher Scientific, USA) at 414 nm.

- **Determination of Total Tannins (as tannic acid) of leek (seeds and leaves):**

Calorimetric analysis was used to measure the total tannins in accordance with the protocol described by A.O.A.C. (1995).

**Fractionation of phenolic and flavonoids of leek (seeds and leaves) by HPLC:**

By following the protocol laid forth by Wu *et al*., (2009) and Soengas *et al*., (2012), the phenolic and flavonoid compounds found in the leek (seeds and leaves) were identified. The analysis was carried out utilizing a Waters ν-bondapak C18 column (3.9 x 300 mm), an automated gradient controller, 510 pumps, a U6K injector, 481 detectors, and 746 data modules in the HPLC system. All samples and mobile phases were purified before HPLC injection by passing them through a 0.45µm Millipore filter (type GV) from Millipore, Bedford, MA. At room temperature (24–27ºC), a mobile phase consisting of water, methanol, and acetic acid (70.0: 29.5: 0.5, Vol: Vol) was used to carry out the elution at a rate of 1.0 mL/min. Triplicate analyses were performed on each sample using 280 nm UV detection.

**Antioxidant activity of leek (seeds and leaves):**

- **Determination of antioxidant activity by DPPH scavenging activity:**

The antioxidant capacity of leeks (leaves and seeds) was determined using DPPH, a compound represented by the chemical molecule 2,2-diphenyl-1-picrylhydrazyl. Abd El-Rehem and Ali (2013) provided the methodology for conducting DPPH scavenging activity testing. The UV-Vis Jenway 6003 Spectrophotometer used to measure the absorption at 517 nm. The half-maximum concentration ($IC_{50}$) of a test substance is that concentration at which the concentration of free radicals is 50% reduced.

These are the steps used to determine the radical scavenging activity against DPPH. The equation for inhibition is: % of Inhibition = [(A-A1/A) × 100]
where A is the control's absorbance and A1 is the sample's absorbance when the sample is present.

**Determination of total antioxidant capacity (TAC) of leek (seeds and leaves):**

The phosphomolybdenum (MoO2P) technique to assess the total antioxidant activity of ethanolic extracts from leek (seeds and leaves) according to Kumar *et al*. (2014). The process relies on the extraction of antioxidant chemicals from leek to reduce molybdenum (Mo VI) to (Mo V). At acid pH, a complex between green phosphate and Mo (V) is then formed, and this is the basis of the test. Then, at room temperature, a TS8560

spectrophotometer (China) was used to measure the solution's absorbance at 695 nm compared to a blank. A blank was prepared using 0.3 ml of methyl alcohol instead of the extract. To measure antioxidant activity, the ascorbic acid equivalent (AAE) was measured in milligrams per gram of extract, with a positive control serving as a reference.

**Anticancer activity of leek (seeds and leaves):**

The National Cancer Institute in Cairo, Egypt, supplied the human colon and breast cell lines Michigan Cancer Foundation-7 and human colon cancer (MCF7 and $HCT_{116}$, respectively). The cancer cells were grown in a particular medium that included $HCT_{116}$ and MCF7 cells, along with 10% FBS, 100 U/ml penicillin, 100 µg/ml streptomycin, and 2 ml of glutamine. The cells were then incubated at 37 0C for one day with 5% carbon dioxide in the air, according to El-Hadidy *et al*. (2020).

**Statistical analysis:**

The statistical significance of the standard deviation among groups was determined by conducting an analysis of variance (ANOVA) in one direction. Using SPSS software (Version 16; SPSS Inc., Chicago, USA) (McCormick and Jesus, 2017).

**Density Functional Theory (DFT):**

Computational chemistry approaches are highly effective tools for investigating the structure, molecular characteristics, and antioxidant capabilities (Atish et al., 2022; Bienfait et al., 2022). The density function theory (DFT) and B3LYP approach was employed as described by Becke, (1993). Software packages such as Gaussian 16, Chemcraft b 68, Gaussi view 6.0, and ISIS draw were used for all calculations. As previously stated by Schlegel *et al*. (2009) B3LYP/6-311G (d,p) was used to optimize the molecular geometries of all the compounds under study. The optimization of the geometry does not include any symmetry requirements (El-Hadidy *et al*., 2020).

## RESULTS AND DISCUSSION

**Chemical composition of leek (seed and leaves):**

The mean values of chemical composition (fat, protein, crude fiber, ash, and carbohydrates) of the powder of leek (seeds and leaves) were shown in Table (1).

The seeds were a good source of fat, and protein, whereas the leaves were a good source of crude fiber and ash. It was obvious from Table (1) that the leek seeds contain relatively high amounts of protein (25.40 ±1.62g/100g) and crude fat (11.37±2.21 g/100g) but low fiber (8.95±1.01 g/100g) and ash (5.11±0.85 g/100g), while the leaves contain a high amount of crude fiber (22.40±2.36g/100g) and ash (17.10±1.52g/ 100g) as well as low levels of protein and fat (14.11±1.44 g/100g and 5.42 ±1.18 g/100g, respectively). Both leek seeds and leaves contain high amounts of carbohydrates (49.17±5.69 g/100g and 40.97±6.5g/100g, respectively). El-Khabery *et al*. (2016) and Abd El-Rehem and Ali (2013) reported that the Egyptian leek leaves had a high amount of total carbohydrates and crude protein, while crude fat was the lowest. Moreover, the powder of leek seeds had a high content of carbohydrates and protein but had a low content of ash.

**Table (1). Chemical composition of leek powder (seed and leaves) (g/100g on dry weight basis).**

| Constituents | Leek seed (g/100 g) | Leek leaves (g/100 g) |
|---|---|---|
| Ash | 5.11± 0.85 | 17.10 ±1.52 |
| Crude protein | 25.40 ±1.62 | 14.11±1.44 |
| Total carbohydrates | 49.17 ± 5.69 | 40.97 ± 6.5 |
| Crude fiber | 8.95 ±1.01 | 22.40 ± 2.36 |
| Crude fat | 11.37 ± 2.21 | 5.42 ±1.18 |
| Moisture | 9.30 ±1.03 | 12.65 ± 0.15 |

* Each value represents the means ± SD.

**2. Determination of Phytochemical in leek (seeds and leaves):**

**a) Total phenols in leek (seed and leaves):**

It is clear from Table (2) that the leek leaves had the highest content of phenolic compounds (210±7.5mg GAE/100g) and leek seeds had the lowest content of phenolic compounds (160±5.2mg GAE/100g). Results showed that phenolic compounds (PCs) might contribute directly to the antioxidant action. Kavalcová *et al*. (2014) found that total phenolic compounds in leek ranged from 210.67 to 254.58 mg/kg. While Bernaert *et al*. (2012) reported that total phenolic compounds in fresh leek ranged from 5 to 15 mg GAE/g on dry weight.

**b) Total flavonoids in leek (seed and leaves):**

Data in Table (2) indicated that the leek leaves had the highest content of flavonoid (570±1.2mg/100g) and the leek seeds had a low content of flavonoid (340± 8.3 mg/100g). Also, leaves had significantly higher total flavonoid content than the seeds.

**c) Total alkaloid contents (TAC) of leek (seed and leaves):**

Alkaloids were one of the most important groups of naturally occurring organic compounds with numerous pharmaceutical and medicinal uses. The total alkaloid content of leek leaves (670±1.8 mg/100g) was higher than leek seeds (480±1.6mg/100g) (Table 2). This agrees with Monika and Sakthi (2018) who found that alkaloid compounds were found abundantly in leek.

**d) Total tannins contents (TTC) of leek (seed and leaves):**

Tannins were defined as antinutrients of plant origin because they can precipitate proteins, inhibit digestive enzymes, and decrease the utilization of vitamins and minerals. On the other hand, tannins had also been considered "health-promoting" components in plant-derived foods and beverages. The data were tabulated in Table (2) illustrated that, the leek leaves and seeds had a high content of tannins (556.90±0.52mg TAE/100g) and (415.10± 0.47mg TAE/100g) respectively. Ben-Arfa *et al.* (2015) reported that total tannin in Tunisian leek ranged from 3.47 to 7.62mg.

**Table (2): Total phenols, total flavonoids, total alkaloids and total tannins of leek (seeds and leaves).**

| Plant name | Total phenols (mgGAE/100 g) | Total flavonoids (mg QE /100 g) | Total Alkaloids (mg /100 g) | Total Tannins (mg TAE/100g) |
|---|---|---|---|---|
| Leek leaves | 210± 7.5 | 570± 1.2 | 670±1.8 | 556.90 ±0.52 |
| Leek seeds | 160± 5.2 | 340± 8.3 | 480±1.6 | 415.10 ±0.47 |

**Each value represents the means ± SD GAE: Gallic acid equivalent.** QE: Quercetin equivalent. TAE: tannic acid equivalent.

**d) Determination of Fatty acids in leek (seeds):**

The data in Table (3) showed that leek seeds contained a low concentration of SFA (19.30±0.088%). Moreover, leek seeds had a high level of USFA (80.70 ±0.077%) and had a low level of omega-3. Nehdi *et al.* (2020) found that leek seed oil was rich in unsaturated fatty acids (89.42 %).

**Table (3): Saturated and unsaturated fatty acids percentage in leek seeds.**

| Saturated fatty acids | | Unsaturated fatty acids | |
|---|---|---|---|
| Name of fatty acid | leek seeds | Name of fatty acid | leek seeds |
| | Area Sum % | | Area Sum % |
| Myristic acid | 0.14 ±0.011 | Palmitoleic acid | 0.19 ±0.011 |
| Pentadecanoic acid | 0.11 ±0.011 | Oleic acid | 21.51 ±0.011 |
| Palmitic acid | 14.13 ±0.011 | Linoleic acid | 57.84 ±0.011 |
| Margaric acid | 0.1 ±0.011 | Linolenic acid | 0.59 ±0.011 |
| Stearic acid | 3.98 ±0.011 | cis-11-Eicosenoic acid | 0.46 ±0.011 |
| Behenic acid | 0.18 ±0.011 | DHA | 0.0 |
| Lignoceric acid | 0.29 ±0.011 | EPA | 0.11 ±0.011 |
| Arachidic acid | 0.38 ±0.011 | Total | 80.70 ±0.077 |
| Total | 19.30 ±0.088 | | |

Each value represents the means ± **SD**

**3. Fractionation of phenolic and flavonoids by HPLC of leek (seeds and leaves):**

Data in Table (4) revealed that both non-flavonoids and flavonoids content were relatively high in ethanol extracts (70%) from leek (seeds and leaves). The leek seeds extract contained relatively high amounts of polyphenol compounds like Myricetin (122.24±1.4mg/100g), Vanillic acid (107.10±1.3mg/100g), and other polyphenols compounds and less concentration of Ferulic acid (3.22±0.05mg/100g), Pyrogallol (3.34± 0.04mg/100g) and Caffeic acid (3.61± 0.05 mg/100g). The polyphenols values in the current study were different from Abd El-Rehem and Ali (2013) which might be due to the differences between locations, humidity or soil salinity.

The majority of phenolic compounds in leek leaves extract were Catechol Kaempferol followed by Benzoic acid Ellagic, Rutin, Myricetin and Rosemarinic (Table 4). The values of phenolic acids and flavonoids in the current study were agreed with Abd El-Rehem and Ali (2013) who found that phenolic compounds such as flavonoids and phenolic acids were found abundantly in leek leaves, but there were differences in some concentrations which might be due to the differences between locations and in growing conditions, including temperature, humidity or drought and characteristics of the soil, and salinity (Meot-Duros and Magne, 2009).

**Table (4): Polyphenolic fractions in leek seeds and leaves by HPLC (mg/100g).**

| Phenolic and Flavonoids compounds | Leek seeds | Leek leaves | Phenolic and Flavonoids compounds | Leek seeds | Leek leaves |
|---|---|---|---|---|---|
| **Syringic acid** | **5.37±0.06** | **3.29± 0.06** | **Caffeic acid** | **3.61± 0.05** | **---** |
| **Gallic acid** | **---** | **2.40± 0.03** | **Vanillic acid** | **107.10± 1.3** | **7.54± 0.081** |
| **Pyrogallol** | **3.34± 0.04** | **6.18± 0.05** | **Ferulic acid** | **3.22± 0.05** | **2.91± 0.035** |
| **Myricetin** | **122.24± 1.4** | **26.74± 0.24** | **Ellagic acid** | **4.40± 0.06** | **34.53± 0.27** |
| **Quercetin** | **90.42± 1.2** | **---** | **O– Counmaric acid** | **8.59± 0.09** | **---** |
| **Cinnamic acid** | **---** | **4.74± 0.04** | **Benzoic acid** | **16.60± 0.11** | **36.81± 0.4** |
| **Catechol** | **97.22± 1.1** | **403.03± 3.8** | **Salicylic acid** | **17.38± 0.11** | |
| **Kaempferol** | **76.81± 0.83** | **97.79± 0.94** | **Rutin** | **---** | **30.10± 0.28** |
| **Caffeine** | **17.85± 0.07** | **---** | **Chlorogenic acid** | --- | 4.27± 0.04 |
| **P-OH-benzoic acid** | **14.97± 0.07** | **---** | **P– Counmaric acid** | **---** | **3.52± 0.044** |
| **Rosemarinic** | **---** | **21.53± 0.18** | | | |

Each value represents the means ± **SD.**

**4. Antioxidant properties of leek (seeds and leaves):**

**a. DPPH radical-scavenging activity of leek (seeds and leaves):**

DPPH was a common abbreviation for the organic chemical compound 2,2-diphenyl-1-picrylhydrazyl. It was a well-known radical and a trap (scavenging) for other radicals. Therefore, the rate of reduction of the chemical reaction upon the addition of DPPH was used as an indicator of the radical nature of that reaction (Gulcin and Alwase, 2023; Mathangi and Prabhakaran, 2013). Results of the DPPH scavenging activity of leek (seeds and Leaves) represented in Figure (1) and Table (5) revealed that the leek seeds extract had relatively high value ($IC_{50}$=11.24± 0.1mg/ml) indicating that, the leek seeds had relatively low value of free radical scavenging activity (antioxidant activity), where the relation between the value of $IC_{50}$ and antioxidant activity was an inverse relationship. On the other hand, the leek leaves extract had relatively low value ($IC_{50}$=7.71±0.081mg/ml) indicating that the leek leaves extract had a high value of free radical scavenging activity (antioxidant activity) which could be attributed to the presence of some compounds with high levels such as catechol in leek leaves that have antioxidant activity. The higher of the content of the total phenolic compounds indicated the stronger antioxidant activity (Baardseth *et al*., 2010). Zafar *et al*. (2016) reported that catechol groups were highly reactive and active against the free radicals as a single catechol group could scavenge two radicals at the same time.

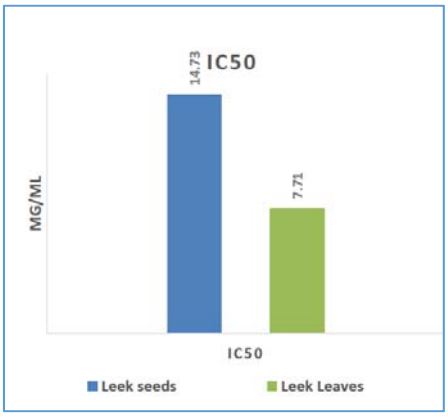



**Fig. (1). Free Radical-scavenging activity of leek (seed and leaves).**

**b. Total antioxidant capacity (TAC) of leek (seeds and leaves):**

The phosphomolybdenum method is an assay based on the reduction of molybdenum (MoVI to MoV) by the antioxidant compounds and subsequent formation of a green phosphate/Mo(V). It was quantitative since the antioxidant activity was expressed as the number of equivalents of ascorbic acid (AA) per g of dry extract. From table (5) leek leaves extract had a higher total antioxidant capacity (682.70± 3.82 mg/100g) than leek seeds extract (91.66± 0.86 mg/100g). These results were agreed with the DPPH radical-scavenging activity of leek (seeds and leaves). This illustrated that the leek leaves were strong antioxidant agents, and this agreed with Benedé *et al*. (2019). From previous results. It was clear that DPPH radical-scavenging activity, total antioxidant capacity, total alkaloid contents, total tannins contents, flavonoids, and polyphenols analysis that leek leaves are powerful antioxidant agent than leek seeds.

**Table (5). Free radical-scavenging activity of leek (seed and leaves) extracts by DPPH and total antioxidant capacity of leek (seeds and leaves).**

| Plant name | $IC_{50}$ | Total antioxidant capacity (TAC) (mg AAE /100g) |
|---|---|---|
| Leek leaves | 7.71± 0.081 | 682.70± 3.82 |
| Leek seeds | 11.24± 0.1 | 91.66± 0.86 |

Each value represents the means **± SD.**
AAE: Ascorbic acid equivalent.

**5. In Vitro Anticancer activity of leek (seeds and leaves):**

There are more than 100 types of cancer and types of cancer are usually referred to the organs or tissues where the cancers originated from (like lung cancer starts in cells of the lung, brain cancer starts in cells of the brain, etc.) (Mileo and Miccadei, 2016).

**a) Effect of leek (seeds and leaves) extract on the colon carcinoma ($HCT_{116}$):**

The anticancer activity of the leek leaves and seeds extract has been examined against cancer cell lines that represent colon carcinoma. The data in Table (6) recorded that the leek extract was applied at concentrations ranging from 0.0 to 500µg/ml.

The colon carcinoma in the form of the $HCT_{116}$ cell line exhibited resistance to leek seeds extract and this was demonstrated clearly in the value of $IC_{50}$ which equal 300µg/ml as indicated in Figure (2). The best inhibition results (67.7%) were recorded at high concentration (500µg/ml) of leek seeds extract, while the lowest inhibition activity (24.3%) was recorded at concentration (62.5µg/ml). The colon carcinoma in the form of the $HCT_{116}$ cell line exhibited more resistance to leek leaves extract and this was demonstrated clearly in the value of $IC_{50}$ which equal 313 µg/ml as shown in Figure (3).

**Table (6): Effect of different concentrations of leek leaves (L.L.) and leek seeds (L.S.) extracts on the surviving fraction colon carcinoma ($HCT_{116}$).**

| Plant conc. | $HCT_{116}$ (cells remaining %) | | | | | |
|---|---|---|---|---|---|---|
| | **0** | **62.5 µg/ml** | **125µg/ml** | **250 µg/ml** | **500 µg/ml** | **$IC_{50}$ µg/ml** |
| Leek leaves | 100 % | 76.4± 0.8 | 60.8± 0.6 | 53.1± 0.6 | 39.9± 0.4 | 313±3.2 |
| Leek seeds | 100 % | 75.7± 0.8 | 58.3± 0.6 | 54.2± 0.6 | 32.3± 0.2 | 300±2.9 |

Each value represents the means **± SD.**

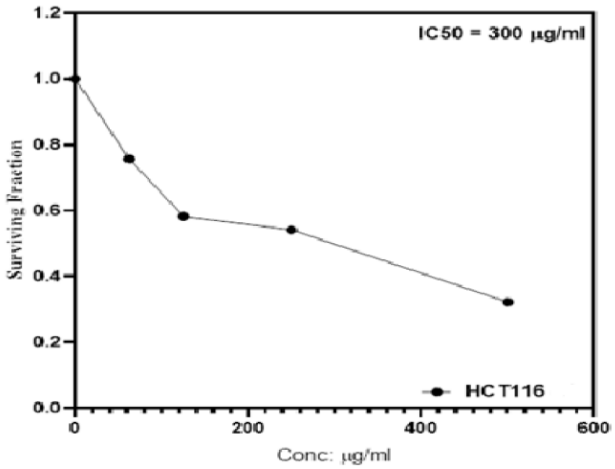



**Fig. (2). Effect of different leek seeds extract concentrations on the surviving fraction of colon carcinoma ($HCT_{116}$).**

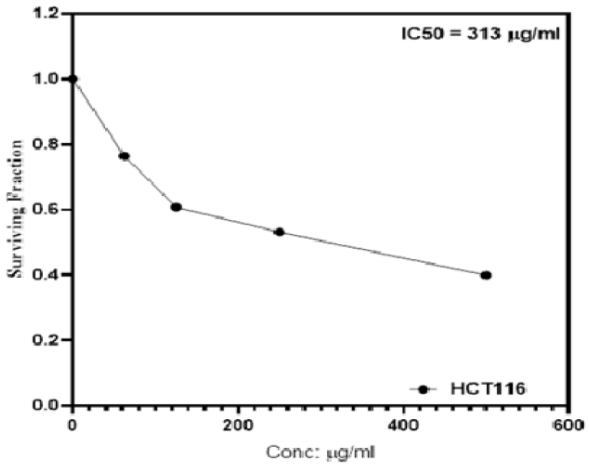



**Fig. (3). Effect of different leek leaves extract concentrations on the surviving fraction of colon carcinoma ($HCT_{116}$).**

**b) Effect of leek (seeds and leaves) extract on breast cancer (MCF7):**

The anticancer activity of the leek leaves and seeds extract has been examined against cancer cell lines that represent breast cancer. The data tabulated in Table (7) recorded that the extract was applied at concentrations ranging from 0.0 to 500µg/ml. The breast cancer in the form of the MCF7 cell line exhibited equal resistance to leek seeds and leek leaves extracts and this was demonstrated clearly in the value of $IC_{50}$ which equal 450µg/ml as in Figures (4 and 5). The best inhibition results (51.8%) were recorded at a high concentration of 500µg/ml, while the lowest inhibition value 22.4 %) was recorded at a low concentration of 62.5µg/ml. In leek seeds extract the best inhibition results (71.4 %) were recorded at a high concentration (500 µg/ml), while the low concentration of 62.5µg/ml produced 22.2 % inhibition value.

The leek could be used as preventive agents for the delay or inhibition of cancer development. Before developing treatment plans, however, it was necessary to consider crucial aspects of the in vivo impacts, such as dose efficacy, molecular changes, bioavailability, effects on healthy cells and long-term exposure.

Flavonoids, albeit to variable degrees, had a well-established antioxidant role that confers many of their health protective functions. However, their anticancer activities were associated with differential effects on ROS level depending on cancer type, cell line, oxidative state of the cell, type (type of flavonoids was very important to match with the type of cancer), and amount of flavonoid used, and duration of exposure. Therefore, by controlling reactive oxygen species (ROS) levels, flavonoids were capable of hindering the initiation, promotion, and progression of cancer via several mechanisms. Nevertheless, these results merit be properly extrapolated to humans to assess the efficacy and safety of these results agreeing with Hasan et al. (2022).

**Table (7): Effect of different concentrations of leek leaves (L.L.) and leek seeds (L.S.) extracts on the surviving fraction breast cancer (MCF7).**

| Plant conc. | MCF7(cells remaining %) | | | | | |
|---|---|---|---|---|---|---|
| | 0 | 62.5 µg/ml | 125µg/ml | 250 µg/ml | 500 µg/ml | $IC_{50}$ µg/ml |
| L.L | 100 % | 77.6± 0.8 | 66.1± 0.7 | 58.8± 0.6 | 48.2± 0.5 | 450±4.2 |
| L.S | 100 % | 78.8± 0.8 | 75.5± 0.8 | 55.9± 0.6 | 28.6± 0.3 | 450±4.2 |

Each value represents the means ± **SD.**

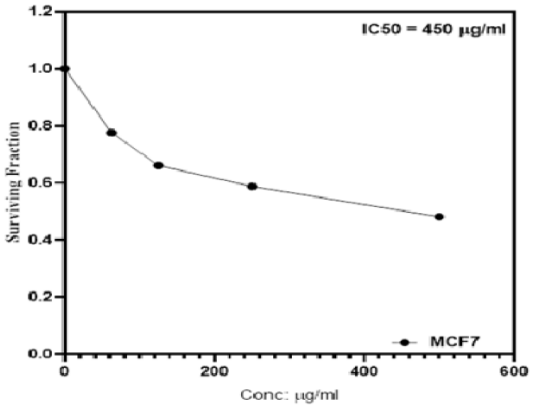



**Fig. (4). Effect of different leek leaves extract concentrations on the surviving fraction of breast cancer (MCF7).**

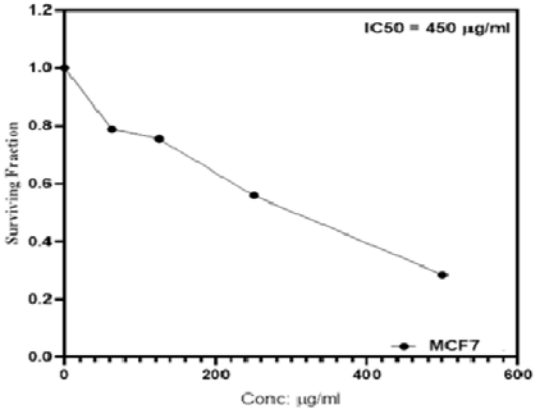



**Fig. (5). Effect of different leek seeds extract concentrations on the surviving fraction of breast cancer (MCF7).**

**7. Geometry optimization of some polyphenols and phenols in leek (seeds and leaves):**

Detailed knowledge of electronic and structural properties of antioxidant compounds was very importance in describing their scavenging behavior. Hence, several initial geometries of investigated compounds had been selected to undergo a full optimization. Geometry optimization was carried out under the B3LYP/6-311G (d,p) level basis set of Gaussian (09). The main structural features in antioxidants were the presence of -SH/-OH group either in the parent molecule or in their reduced form. Schemes (1&2) show the chemical structures and nomenclature of some polyphenols as (benzoic acid, caffeic acid, catechol, galic

acid, pyrogallol, and quinone, resveratrol and vanillic acid) molecules. The optimized structures, the vector of the dipole moment, net charge and numbering system of these non-flavonoids components were shown in Figures (7-10). The bond length of some non-flavonoids was tabulated in Table (10). The ground state parameters (the ionization potential (I), electron affinity (A), chemical potential (Ц), electronegativity ($\chi$), total energy (ET), energy gap (ΔE) and dipole moment (μ)) of the studied polyphenols molecules were listed in Table (11).

According to the literature, three primary antioxidant mechanisms for scavenging of phenolic antioxidants had been reported.

(1) hydrogen atom transfer (HAT).

(2) stepwise electron-transfer-proton-transfer (ET-PT).

(3) sequential proton-loss-electron-transfer (SPLET).

HAT mechanism was energetically more desirable than SPLET pathways regarding the antioxidant nature of the studied compound, where HAT mechanism depend on the nature of (O-H) bond and could be measure by BDE or net charge and bond length of O-H bond while (ET-PT) mechanism could be measured by ionization potential (IP). From Tables (10 & 11), Schemes (1 & 2) and Figures (7-10) we note that:

a) The differences in bonds lengths of (O-H) in the studied non-flavonoids were very low except one bond (O-H) in Catechol and Pyrogallol.

b) Both Resveratrol and Pyrogallol had low ionization potential (IP) where the lower IP value cause the higher antioxidant activity.

c) Although Caffeic acid and Galic acid had relative high ionization potential (IP), they had high dipole moment (μ) that was mean, they might be had high antioxidant activity in polar solvent as water.

d) The ionization potentials of the studied compounds were in following order (descending order);

Benzoic acid > Galic acid > Quinone > Vanillic acid > Caffeic acid> Catechol > Pyrogallol> Resveratrol.

e) The electronegativity (**X**) of the studied compounds were in following order (descending order);

Benzoic acid > Galic acid > Caffeic acid> Vanillic acid > Quinone > Resveratrol > Catechol > Pyrogallol.

f) Both Catechol and Pyrogallol had low electronegativity (**X**) this was mean they had good antioxidant activity.

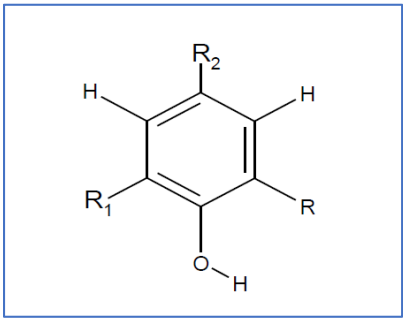
g) The molecular dipole moment represents a generalized measure of bond properties and charge densities in a molecule. It essentially constitutes an index of reactivity, which was very important to define the biological properties particularly related to the interaction with enzyme active sites.

Dipole moment of the studied compounds were in following order (descending order);

Galic acid> Caffeic acid > Pyrogallol> Catechol > Resveratrol > Benzoic acid > Vanillic acid > Quinone in case of neutral compounds.

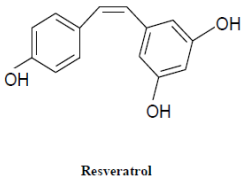
h) From figures (11-15) we note that, the non-flavonoids compounds had number of free radicals might be formed. The order of electron affinity of these compounds could be given as follow (descending order);

Caffeic acid> Galic acid > Benzoic acid > Vanillic acid > Resveratrol> Quinone > Catechol > Pyrogallol. The electron affinity of Caffeic acid and Galic acid were very high, which indicates that these compounds had low electron accepting tendency but high electron donating ability this was mean that, they had good antioxidant activity.

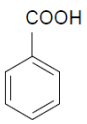



| Nomenclature | R | R1 | R2 | NR |
|---|---|---|---|---|
| **Catechol** | OH | H | H | 2 |
| **Caffeic acid** | OH | H | C2H2COOH | 2 |
| **Gallic acid** | OH | OH | COOH | 3 |
| **Vanillic acid** | H | OCH3 | COOH | 2 |
| **Quinol** | H | H | OH | 2 |
| **Pyrogallol** | OH | OH | H | 3 |

**Scheme 1: Chemical structures and nomenclature of the 6 phenolic (non-flavonoids) compounds at different (R, R1, and R2) and number of free radicals might be formed (NR).**




Resveratrol




Benzoic acid

| Nomenclature | NR |
|---|---|
| Benzoic acid | 1 |
| Resveratrol | 3 |

**Scheme 2. Chemical structures and nomenclature of Resveratrol and benzoic acid and number of free radicals might be formed (NR).**

**Table (10). The bond length of some non-flavonoids.**

| Nomenclature | Position | Bond length | Nomenclature | Position | Bond length |
|---|---|---|---|---|---|
| **Benzoic acid** | O14-H15 | 0.976 | **Pyrogallol** | O10-H11 | 0.975 |
| **Caffeic acid** | O20-H21 | 0.976 | | O12-H13 | 0.969 |
| | O12-H13 | 0.97 | | O14-H15 | 0.972 |
| | O10-H11 | 0.975 | **Quinone** | O11-H12 | 0.974 |
| **Catechol** | O13-H14 | 0.969 | | O13-H14 | 0.974 |
| | O11-H12 | 0.975 | **resveratrol** | O9-H10 | 0.971 |
| **Galic acid** | O9-H10 | 0.976 | | O16-H17 | 0.971 |
| | O11-H12 | 0.975 | | O28-H29 | 0.972 |
| | O13-H14 | 0.971 | **Vanillic acid** | O10-H11 | 0.977 |
| | O16-H17 | 0.974 | | O14-H15 | 0.976 |

**Table (11). The ionization potential (I), electron affinity (A), chemical potential (Ц), electronegativity ($\chi$), total energy (ET), Energy gap (ΔE) and dipole moment (μ) of some non-flavonoids.**

| Component | Benzoic acid | Caffeic acid | Catechol | Galic acid | Vanillic acid | Resveratrol | Pyrogallol | Quinone |
|---|---|---|---|---|---|---|---|---|
| I (eV) | 7.438 | 6.315 | 6.047 | 6.9718 | 6.3849 | 5.5925 | 5.8867 | 6.8511 |
| A (eV) | 1.7987 | 2.1413 | 0.1981 | 1.9609 | 1.5916 | 1.5263 | -0.0416 | 0.7363 |
| $\chi$ (eV) | 4.61835 | 4.22815 | 3.12255 | 4.4663 | 3.98825 | 3.5594 | 2.92255 | 3.7937 |
| Ц (eV) | -4.61835 | -4.2282 | -3.1226 | -4.466 | -3.9883 | -3.5594 | -2.9226 | -3.7937 |
| ET (a.u) | -420.8103 | -648.644 | -382.680 | -646.46 | -610.546 | -766.346 | -457.8874 | -382.6765 |
| μ (D) | 2.1272 | 6.3244 | 2.9529 | 7.2115 | 1.7763 | 2.4536 | 3.6183 | 0.0082 |

$\chi$ =(I+A)/2 (electronegativity) where I and A are ionization potential and electron affinity, and I= -$E_{HOMO}$ while, A= -$E_{LUMO}$, respectively and the total static dipole moment (μ).

## - Frontier molecular orbital theory:

The frontier molecular orbital energies, $E_{HOMO}$ and $E_{LUMO}$ were also very crucial factors of molecular electronic structure. The antioxidant activity had been found to be related to the distributions of frontier orbitals. The lower of the $E_{HOMO}$ implies that the molecule had the electron donating ability, while higher the $E_{HOMO}$ implies that the molecule was a good electron donor. The $E_{LUMO}$ represents the ability of a molecule to accept electron.

The frontier orbital calculated for the studied neutral compounds at the level of B3LYP/6-311G (d,p) in the gas phase, electron density distribution of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) was given in Figures (11-15) and the frontier orbital energy was also indicated in Table (12). The active site could be demonstrated visually by the distribution of frontier orbital. Figures (11-15) shows that the electron densities of the HOMO were localized over benzene ring in (Caffeic acid, Benzoic acid, Vanillic acid, Resveratrol, Quinone, Catechol and Pyrogallol) except gallic acid, So O-H bonds and C-H in (COOH) groups be the preferred attack site for free radicals.

It could be seen from Table (12) that Benzoic acid possesses the lowest $E_{HOMO}$ (-7.438 eV) among the studied compounds, while Resveratrol owns the highest $E_{HOMO}$ (- 5.5925 eV). Based on our calculations, the trend for computing $E_{HOMO}$ was scarcely different from that of BDE [58], correspond to the arrangement (ascending order); Benzoic acid < Galic acid < Quinone < Vanillic acid < Caffeic acid< Catechol < Pyrogallol < Resveratrol.

From the above Resveratrol should be the strongest electron donor (had good antioxidant activity) while Benzoic acid the weakest electron donor (had low antioxidant activity).

Another parameter to be given importance was the energy gap ($E_{gap}$) of these three compounds. The lower $E_{gap}$, the easier the easier the electrons inspire give vigorous evidence to the antioxidant action. The low magnitude of the band gap energy indicates that the compounds could be a highly reactive system. The order of energy gap of these compounds could be given from Table (12) as follow (descending order); Quinone > Pyrogallol> Catechol > Benzoic acid > Galic acid > Vanillic acid > Caffeic acid > Resveratrol. This mean that, Resveratrol and Caffeic acid were the highest active compounds than others while quinone and pyrogallol were the lowest active compounds than the others.

The acquired results (Table 12) display that the antioxidant capability for the Resveratrol had the smallest band gap (energy gap = 3.6313 eV), therefore it was the most having antioxidant molecule according to band gap values. So other investigated molecules, Pyrogallol, Catechol and Caffeic acid were powerful candidates depending on orbital distributions although their band gaps were bigger than others. The molecular descriptors which were I, A, μ and χ values of the studied compounds (Tables 11 and 12) clearly demonstrate that the studied molecules prefer to act as e-donors instead of recipients in the studied.

Generally, from the above result, it was clear that the leek plant leaves had antioxidant properties. They contain highly reactive molecules such as Pyrogallol, Catechol, and Caffeic acid which act as powerful antioxidants. Although the leek leaves had the highest antioxidant activities in this study but, they had lower anticancer effects than purslane (leaves or seeds).

**Table (12). The frontier orbital energy and energy gap of some non-flavonoids.**

| Component | $E_{HOMO}$ | $E_{LUMO}$ | $E_{gap}$ | Component | $E_{HOMO}$ | $E_{LUMO}$ | $E_{gap}$ |
|---|---|---|---|---|---|---|---|
| **Benzoic acid** | -7.438 | -1.7987 | 5.6393 | **Resveratrol** | -5.5925 | -1.5263 | 4.0662 |
| **Caffeic acid** | -6.315 | -2.1413 | 4.1737 | **Pyrogallol** | -5.8867 | -0.0416 | 5.9283 |
| **Catechol** | -6.047 | -0.1981 | 5.8489 | **Quinone** | -6.8511 | -0.7363 | 6.1147 |
| **Galic acid** | -6.9718 | -1.9609 | 5.011 | **Resveratrol** | -5.5925 | -1.5263 | 4.0662 |
| **Vanillic acid** | -6.3849 | -1.5916 | 4.7933 | | | | |

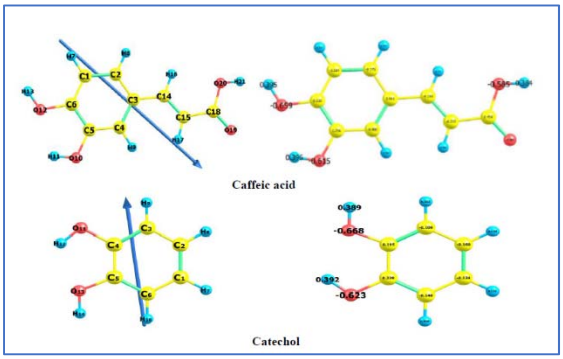



**Fig. (7). Geometry optimization, the vector of the dipole moment, net charge and numbering system of Caffeic acid and Catechol.**

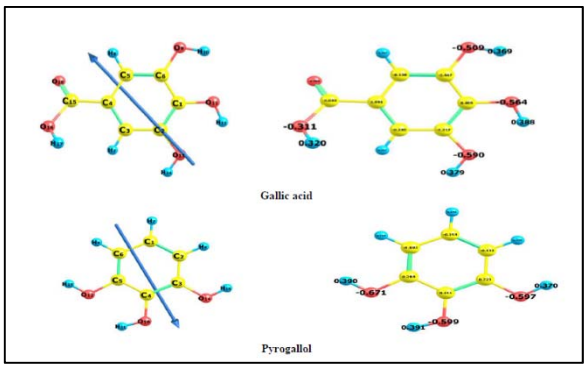



**Fig. (8). Geometry optimization, the vector of the dipole moment, net charge and numbering system of Gallic acid and Pyrogallol.**

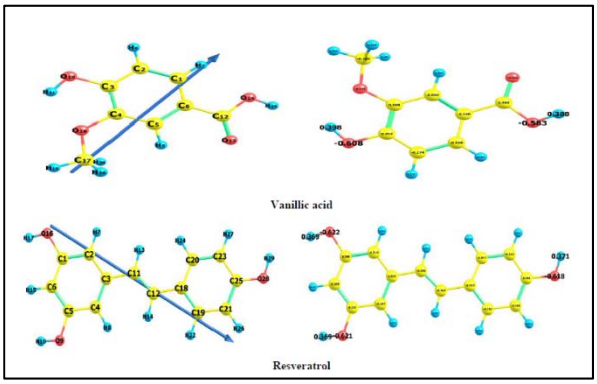



**Fig. (9). Geometry optimization, the vector of the dipole moment, net charge and numbering system of Vanillic acid and Resveratrol.**

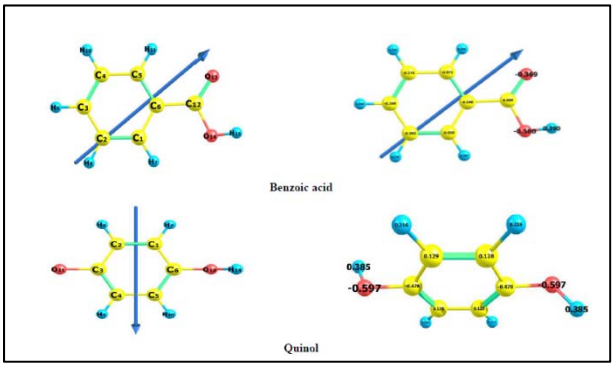



**Fig. (10). Geometry optimization, the vector of the dipole moment, net charge and numbering system of Benzoic acid and Quinol.**

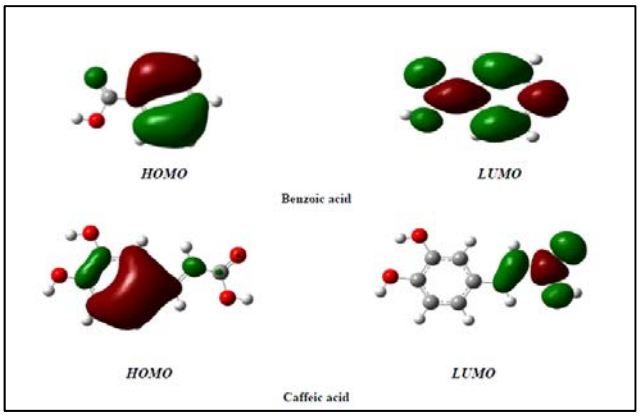



**Fig. (11). The charge density maps of the HOMO and LUMO for optimized structure of Benzoic acid and Caffeic acid.**

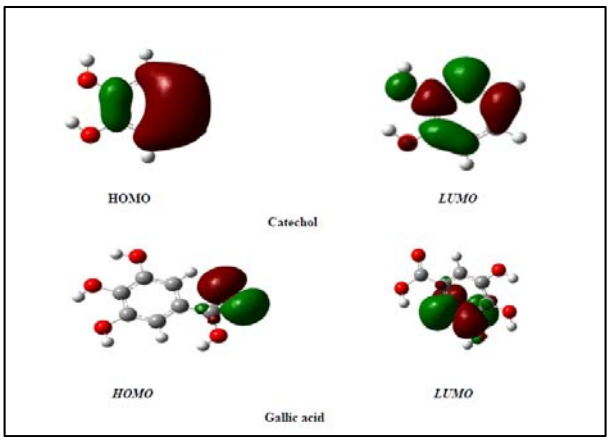



**Fig. (12). The charge density maps of the HOMO and LUMO for optimized structure of Catechol and Gallic acid.**

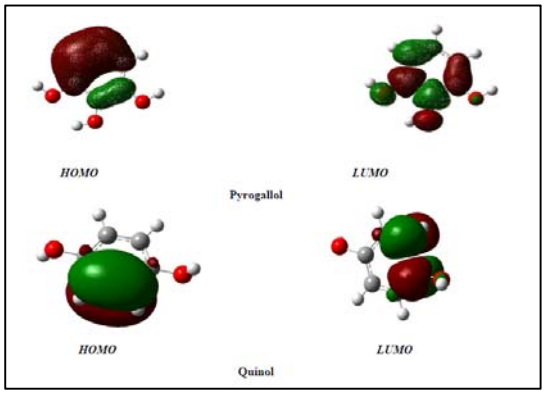



**Fig. (13). The charge density maps of the HOMO and LUMO for optimized structure of Pyrogallol and Quinol.**

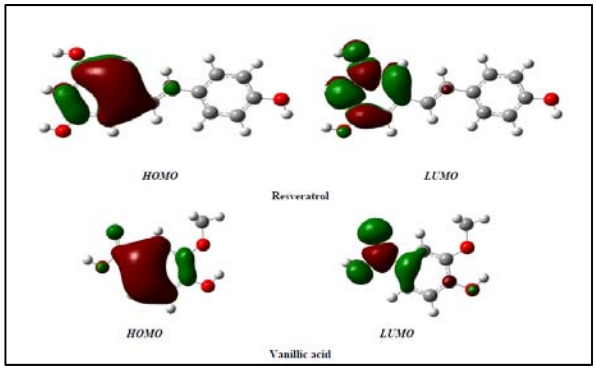



**Fig. (14). The charge density maps of the HOMO and LUMO for optimized structure of Resveratrol and Vanillic acid.**

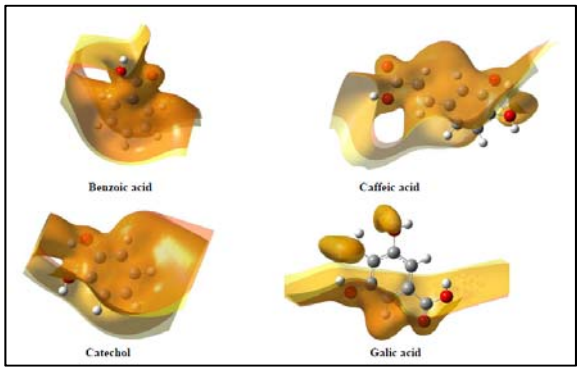



**Fig. (15). Electrostatic potential from total SCF density of Benzoic, Caffeic acid, Catechol and Galic acid.**

**Conclusion:**

The results indicated that the leek leaves have high amount of phenolic compounds (0.21± 0.075g/100g), flavonoids (0.57± 0.12 g/100g), alkaloids (0.67± 0.018 g/100 g) and tannins (556.90 ±0.52 mg tannic acid equivalent/100g). While, the leek seeds have high amount of unsaturated fat acids specially omega-3 and omega -6 about 58% per 100 g unsaturated fat acids.

On the other hand, the leek seeds and leaves have anti-cancer properties against colon carcinoma ($HCT_{116}$) and breast cancer (MCF7).

Density function theory (DFT) showed that Pyrogallol, Catechol, and Caffeic acid have more powerful antioxidants than the other phenolic compounds in this study.

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# تأثير بذور وأوراق الكراث المصري على سرطان القولون والثدي بناءً على نشاطها المضاد للأكسدة و قيم دالة الكثافة (DFT)

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**المستخلص**

الكراث المصري (*Allium ampeloprasum* var. kurrat) له تأثيرات مفيدة على صحة الإنسان ويمتلك خصائص غذائية استثنائية و خصائص قوية مضادة للأكسدة ويمنع نمو الأورام الخبيثة. تهدف الدراسة الحالية إلى دراسة نشاط مضادات الأكسدة والتأثير المضاد للسرطان للمواد الكيميائية النباتية الموجودة فى الكراث مثل المركبات الفينولية والفلافونويدات والعفص والقلويدات في الكراث (البذور والأوراق). أظهرت النتائج أن أوراق الكراث هي مصادر جيدة للرماد (17.10±1.52 جم/100جم) والألياف الخام (22.40±2.36جم/100جم). بينما تعتبر بذور الكراث مصدرًا جيدًا للبروتين (25.40 ± 1.62 جم / 100 جم) والدهون الخام (11.37 ± 2.21 جم / 100 جم). تحتوي أوراق الكراث على مستوى عالٍ من البوليفينول (0.21 ± 0.075 جم / 100 جم)، والفلافونويدات (0.57 ± 0.12 جم /100 جم)، والقلويات (0.67 ± 0.018 جم / 100 جم) والعفص (556.90 ± 0.52 مجم مكافئ حمض التانيك /100 جم). كانت قيم المواد الكيميائية النباتية أعلى في أوراق الكراث عن بذور الكراث. يوجد حمض اللينوليك (أوميغا 6) بنسبة عالية فى بذور الكراث (57.84 ±0.011 جم/100 جم)، وقد وجد ان Myricetin وKaempferol أكثر الفلافونويدات وفرة في بذور الكراث، في حين كان الكاتيكول وحمض البنزويك أعلى الفلافونويدات في أوراق الكراث. أوضحت النتائج ايضا أن أوراق الكراث لديها قدرة إجمالية مضادة للأكسدة أعلى من بذور الكراث. وقد أظهر الكراث تأثيرًا عاليًا مضادًا للسرطان على خلايا سرطان الثدي (MCF-7) وخلايا سرطان القولون ($HCT_{116}$) وفقًا لخلايا سرطان الثدي IC50 على شكل خط الخلايا (MCF-7). أظهرت نظرية دالة الكثافة (DFT) أن البيروجالول والكاتيكول وحمض الكافيك تحتوي على مضادات أكسدة أقوى من المركبات الفينولية الأخرى.

**الكلمات المفتاحية:** المواد الكيميائية النباتية، مضادات الأكسدة، العفص، المركبات الفينولية، الفلافونويدات، الكراث.