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# The encapsulation of the gemcitabine anticancer drug into grapheme nest: a theoretical study

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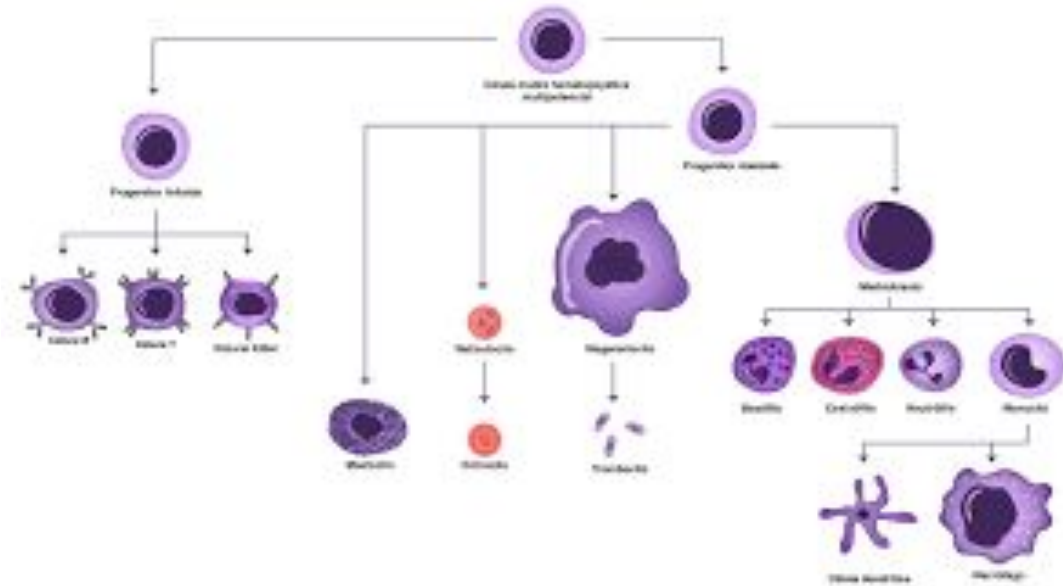
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# INTRODUCCIÓN

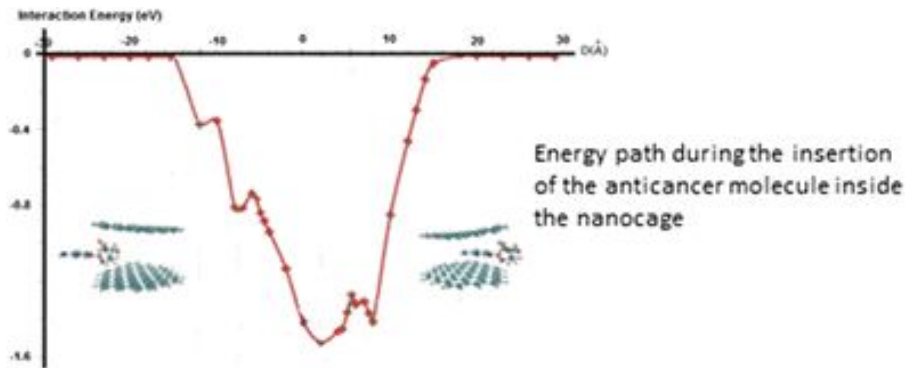
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## Gemcitabina (GEM)

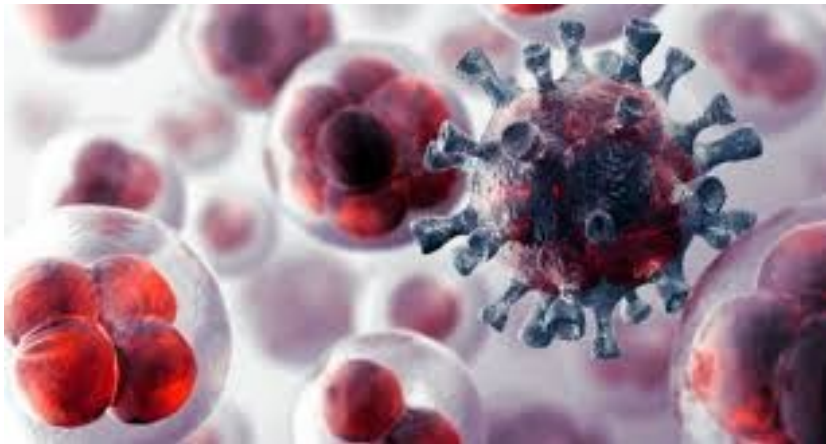
- Agente antitumoral
- Administración limitada
- Posible solución “nanovehículos”



## NANOVECTOR A BASE DE GRAFENO



*“Los nanotubos de carbono es una estrategias prometedora para mejorar el tratamiento del cáncer ya que aumenta su eficacia terapéutica disminuyendo los efectos secundarios”*



## Geometría de las capas de grafeno ( $C_{108}H_{36}$ )

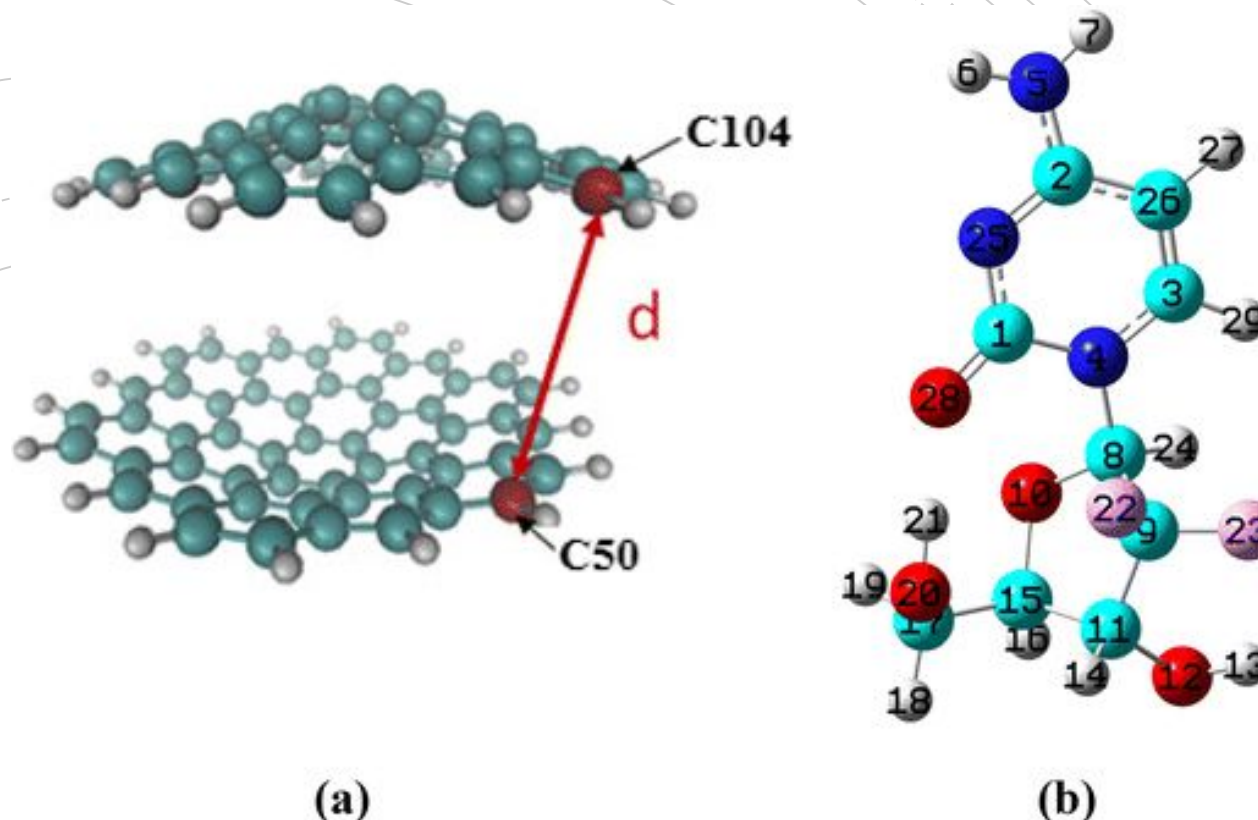


Fig. nº1: (a) Geometry of the graphene layers ( $C_{108}H_{36}$ ) in a nest configuration (C and H atoms are represented as blue and gray balls, respectively). The variable  $d$  represents the interlayer distance and is defined as the distance between the two atoms C50 and C104 shown in red balls. (b) Atom labeling and optimized geometry of gemcitabine (C, O, H, N, and F atoms are represented as cyan, red, white, blue, and pink balls, respectively)

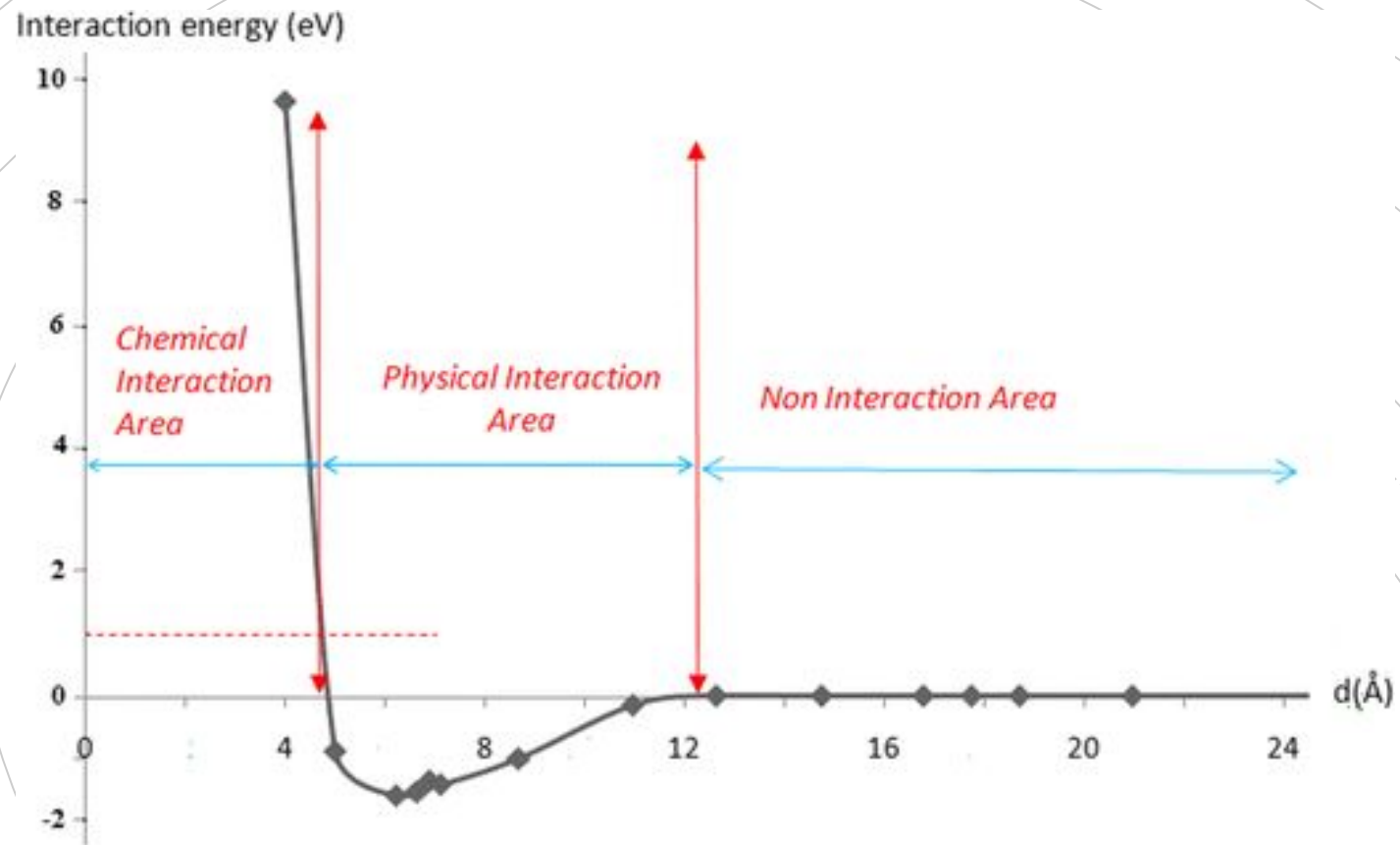
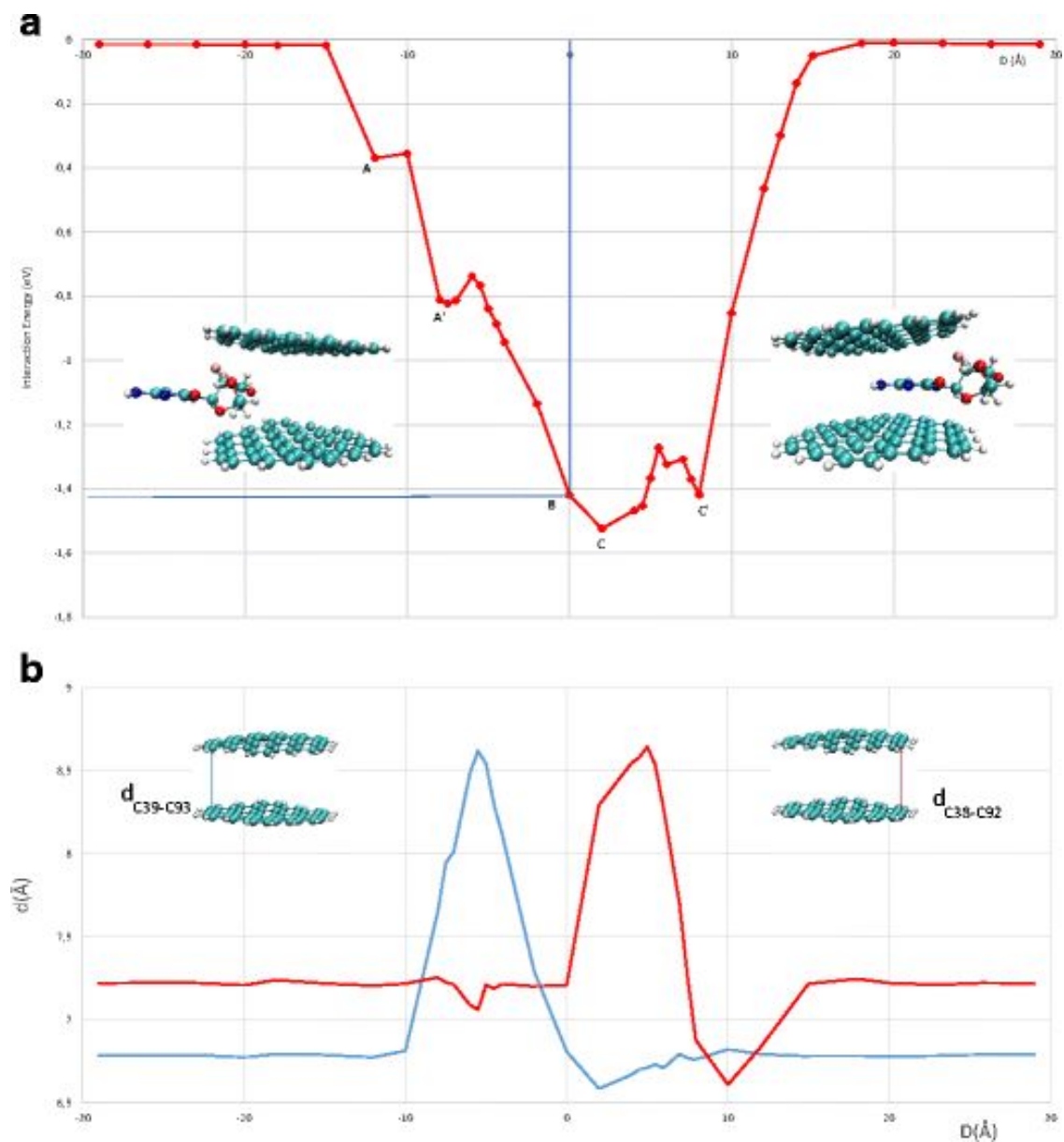


Fig. n°2: (a) Scheme of the hexagonal graphene sheet divided in equidistant family of carbon atoms (shown by different colors) from the center O. (b) Representation of the new coordinate system describing a graphene nest

Fig. n°3: Interaction energy of GEM versus the inter-layer distance  $d$ , defined as the distance between the two atoms C104 and C50 (red bars delimit the different areas of interaction)





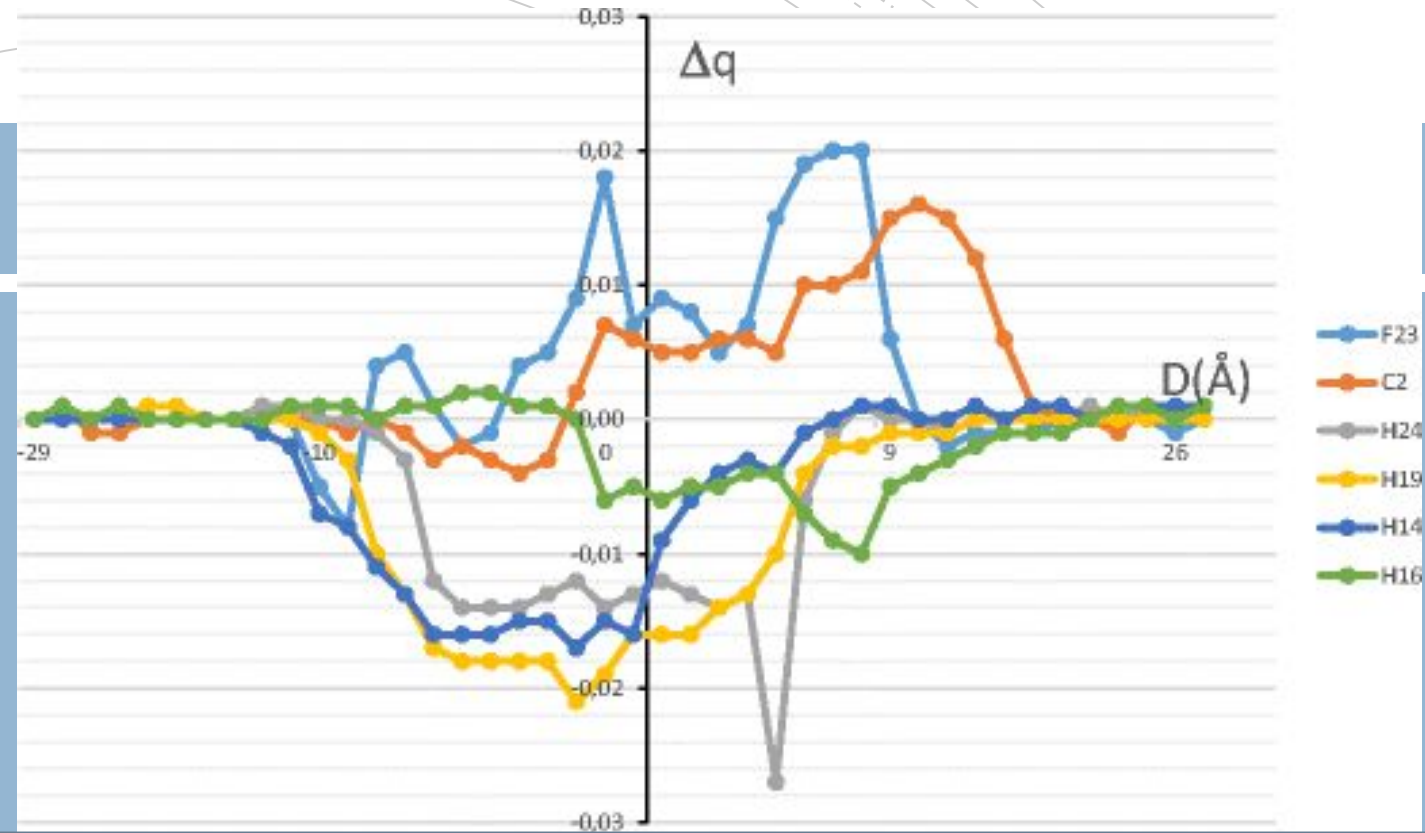


Fig. n°4: (a) Adsorption energy in eV of GEM during its encapsulation inside the nest of graphene and its release from it. (b) Distance C-C as a function of  $D$  (red curve the distance between C38-C92; blue curve the distance between C39-C93)

## CONCLUSIONES

Las interacciones entre una molécula anticancerígena (GEM) y las paredes internas de un sistema compuesto por dos capas de grafeno que forman un nido.

La optimización de varios sistemas se encapsuló determinando la distancia entre capas más favorable para estabilizar el GEM dentro de la cavidad de carbono.

El estudio teórico de la inserción del GEM y su liberación mostró que es posible encapsular y estabilizar las moléculas GEM contra el cáncer entre dos capas de grafeno.