

POM Analysis of Taxol anti-cancer drug: What Derivative is in Perspectives

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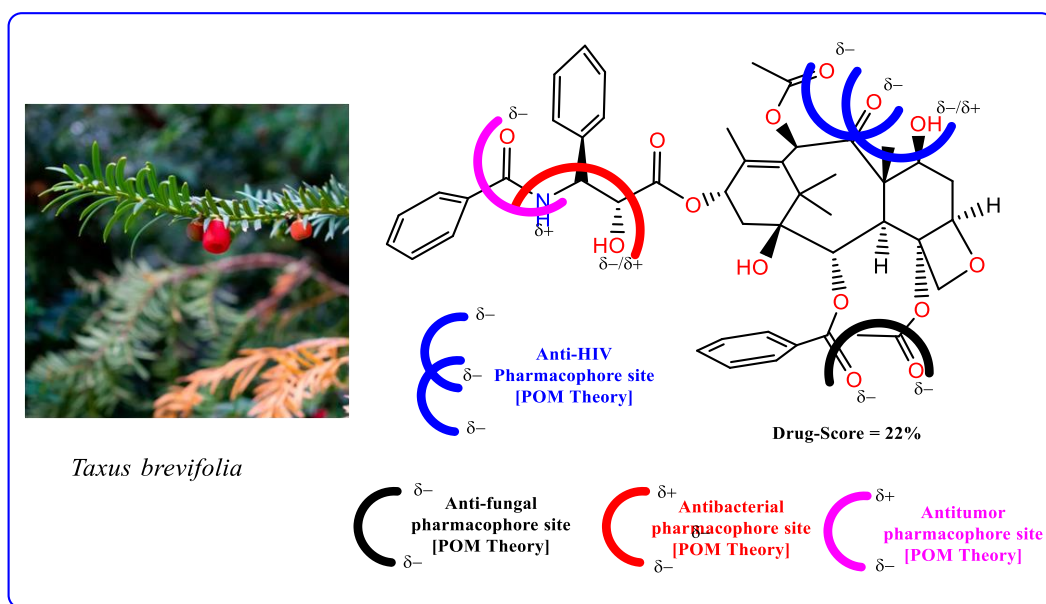
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Graphical Abstract



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1. Introduction

Plants have long been a source of pharmaceutical ingredients (Wani, *et al.*, 1971; Ma *et al.*, 2005; Diass *et al.*, 2021; Latif and Nawaz, 2026), but no natural compound has gained as much fame as Taxol (originally known by its generic name, paclitaxel), both scientifically and in terms of public recognition

(**Figure 1**). Since its development in 1971, multiple uses have been found for it, particularly in the battle against various forms of cancer. Today, Taxol and its derivatives are the most widely marketed anticancer drugs worldwide, generating a turnover profit in excess of three billion dollars annually (Aouzal 2010; Mok, *et al.*, 2009; Chou 2006; Newman et Cragg 2012; Wani, *et al.*, 1971; Davis, *et al.*, 2008).

One of the most important organic molecules today is Taxol, an anticancer compound extracted from yew trees. Although it is a ‘modern’ compound, chemists have been interested in Taxol since the 1990s; however, its structure was determined in 1971.

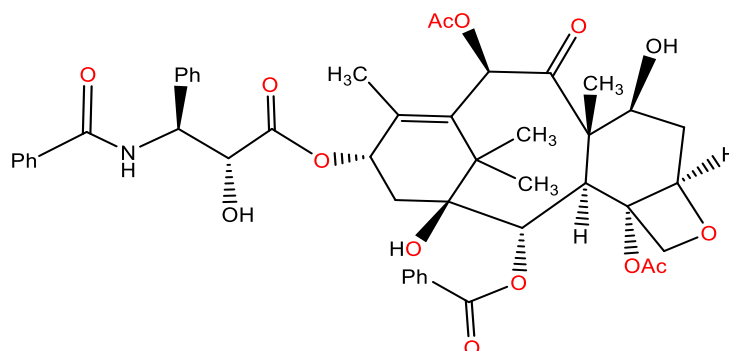


Figure 1. Molecular structure of Taxol.

1200 Scopus articles conducted a bibliometric analysis on Taxol is necessary to get more information about the most published countries and authors as well as the various types of articles and selected journals (Van Eck and Waltman, 2010; Esen *et al.*, 2020; Laita *et al.*, 2024; Nandiyanto *et al.*, 2024; Kachbou *et al.*, 2025; Salghi *et al.*, 2025; Nandiyanto *et al.*, 2026). No one argued with this structure because it was determined by reliable spectroscopic methods—NMR plus an X-ray crystal structure of a derivative. This was not always the case. Go back another 25 years to 1946, when chemists argued about structures incessantly. An undergraduate employing an NMR spectrometer can solve structural problems in a matter of minutes today, whereas this task used to challenge teams of chemists for months and even years. That was only half a century ago.

2. Origin and History

The fascinating story of Taxol took off in 1962 thanks to a joint initiative of the National Cancer Institute and the US Department of Agriculture in the United States, aimed at finding new natural plant extracts that might be effective against cancer cells. In this effort, the western yew (*Taxus brevifolia*) (Schiff, *et al.*, 1979; Koehn et Carter, 2005; Cragg et Newman 2005) was examined, and extracts contained within its bark were found to be cytotoxic against KB cells. Fresh bark samples were collected in 1965 and tested by Monroe Wall and Mansukh Wani at the Research Triangle Institute (Wall, *et al.*, 1966; Wani et Wall, 1969). These extracts were then identified as active against leukemia in mice in

1966. Then, in 1969, a new diterpene was isolated in 0.01% yield of taxol (Batra et Sharma 2013; Wall et Wani, 1995).



Figure 2: Photo of the western yew tree (*Taxus brevifolia*)

Early clinical research on Taxol was not very promising: it showed little efficacy against several types of leukemia and Walker 256 carcinosarcoma, which was extremely difficult to dissolve in water. It could only be extracted from the bark of a slow-growing yew tree (the branches and needles were known to be much less concentrated with Taxol) (Brouwers, et al., 2009; Zhang, et al., 1996). However, research continued at the National Cancer Institute, and in the early 1970s, it was shown to be effective in a mouse model of B16 melanoma (Perdue 1982). Interest in Taxol grew considerably following Susan Horwitz's discovery in 1979 of its mechanism of action: it blocks the duplication of cancer cells by interfering with microtubules, a first at that time. Preclinical and toxicological research was completed in 1982, while clinical trials began in 1984 (Weaver, 2014; Ma, et al., 2025). In 1992, the Food and Drug Administration (FDA) approved the use of Taxol for the treatment of ovarian cancer⁶, followed by its approval for breast cancer⁷ in 1994. Its clinical application was subsequently extended to Kaposi's sarcoma as well as certain types of lung cancer, sometimes in combination with other substances such as cisplatin (Vu Thanh, et al., 2025). Despite its remarkable effectiveness, Taxol had one major drawback: its availability. Indeed, it takes at least 1,000 trees to produce one kilogram of taxol. And a yew tree takes approximately 200 years to reach its adult size. A lively controversy has also arisen between environmentalists and industrialists concerning the risk posed by the exploitation of yew forests in the western United States. Other sources of Taxol have therefore been explored. It is thanks to the cooperation between Rhône-Poulenc Santé and the Institute of Chemistry of Natural Substances in Gif-sur-Yvette that Taxotere was discovered (Schiltz 2005).

3. Structure and Derivatives

Taxol is part of the large taxane family, which includes more than 300 compounds (Gottesman, et al., 2002). The vast majority of taxanes have a tricyclopentadec-11(12)-enic diterpene skeleton. Taxol

(paclitaxel) has several derivatives that have been developed to improve its pharmacological properties, solubility, or reduce its side effects. The main derivatives of Taxol are as follows:

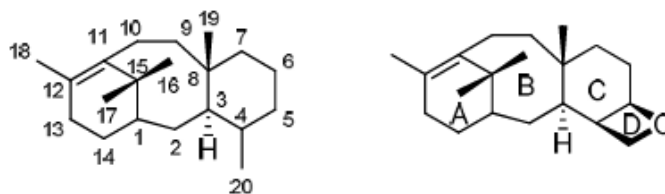


Figure 3: The main structure derivatives of Taxol

4. Chemical Structure

Paclitaxel is a di-terpene secondary metabolite that belongs to the taxoid subclass. Taxol has the following chemical formula: 5 beta, 20-epoxy-1,2 alpha, 4,7 beta, 13 alpha-hexahydroxytax-11-ene-9-one 4,10-di acetate benzoate of (2R, 3S) -N-benzoyl-3-phenylisoserine. It is characterized by the presence of 11 asymmetric centres. Its chemical formula is $C_{47}H_{51}NO_{14}$, and its expanded representation is shown in the figure below.

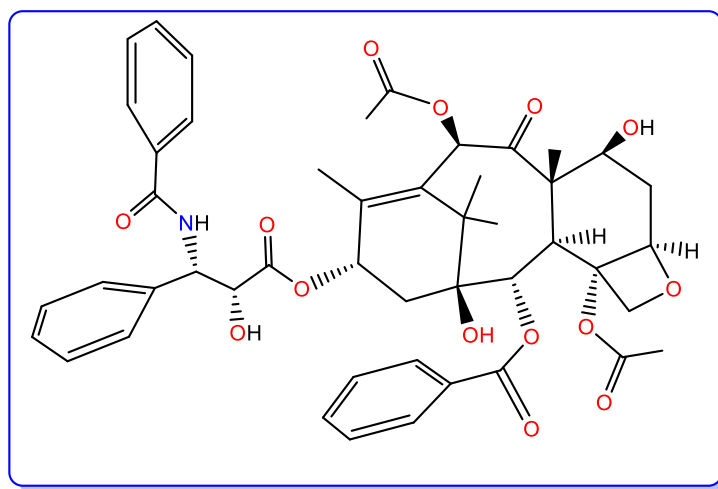


Figure 4: Developed structure of Taxol

Paclitaxel's composition is based on the combination of a complex taxane ring with an oxetane ring at C-4 and C-5, esterified at C-13. According to Rousset (1996), the relative molecular mass is 853.9 daltons. Following an isolation and purification process, Paclitaxel appears as a white to creamy-white powder with low hygroscopicity. Paclitaxel, which does not dissolve in an aqueous environment, finds its solubility in various organic solvents such as methanol, ethyl acetate and acetonitrile. It is not ionizable and therefore does not have a pKa or buffer capacity. Due to its insolubility in aqueous media, the pH could not be determined. On the other hand, the n-octanol/buffer pH 4 partition coefficient, carried out at 24 °C, gives a $c\text{Log}P$ value of 3.7, confirming the very high lipophilicity of this molecule.

5. Extraction of Taxol

Taxol extraction is performed using different methods: dry matter is mixed with methanol to isolate taxol, followed by purification treatments, according to the method described by Vallata and colleagues. For extraction from 30-day-old calli, the calli are dried at 40 ± 2 °C to constant weight, then 0.2 g of dry calli are homogenized with 10 mL of methanol, filtered and evaporated under vacuum at 50 ± 2 °C, before being redissolved in 4 mL of methanol for analysis. For intracellular taxol, 0.2 g of fresh cells are mixed with 10 mL of methanol for 40 minutes, homogenized, filtered, and then evaporated under vacuum at 50 ± 2 °C, with the residue then dissolved in 2 mL of methanol for analysis by HPLC. The extraction of extracellular taxol involves mixing 2 mL of culture medium with dichloromethane (CH_2Cl_2), separating the organic and aqueous phases by decantation, evaporating the solvent at 35 ± 2 °C, and then redissolving the residue in 2 mL of methanol before analysis. Finally, the quantification of taxol in all extracts is carried out by high-performance liquid chromatography (HPLC), following a specific protocol developed by Vallata and his team, allowing the precise determination of taxol content (Havrilesky, *et al.*, 2003).

6. Total synthesis of Taxol:

Many groups have investigated the synthesis of Taxol from more accessible and sustainably sourced taxanes, such as 10 DAB. As mentioned earlier, the latter served as the basis for Potier and Greene's first semi-synthesis of Taxol in 1988. 10DAB is specifically protected by baccatin III, then linked to the side chain by DPC. Taxol is then obtained by hydrolysis (Schiltz 2005).

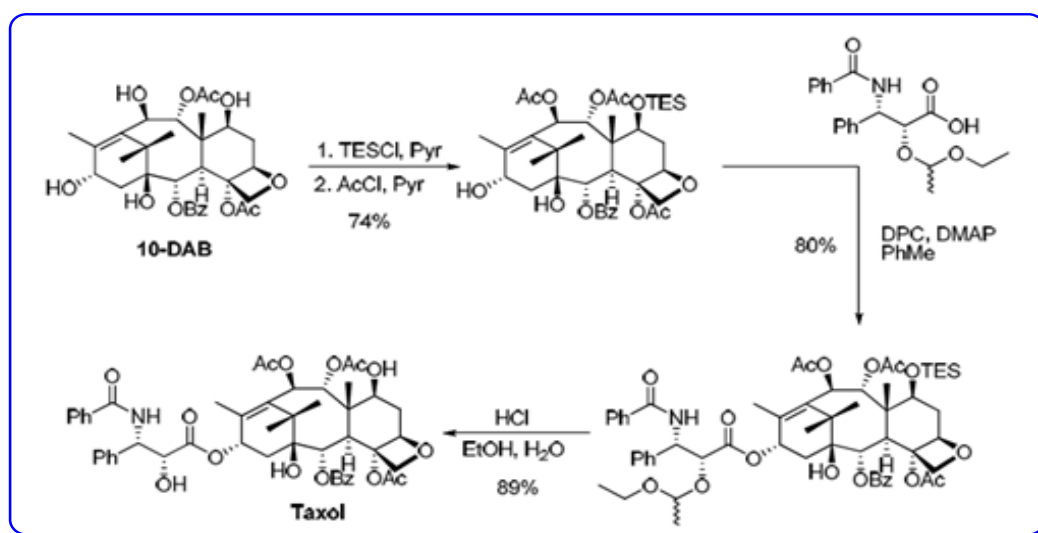


Figure 5: Example of the synthesis of Taxol (Nicolaou, *et al.*, 1994)

7. Activities and applications

Taxol binds to microtubules, stabilizing their structure and preventing their depolymerization, even in the presence of factors that normally promote this process (such as calcium or low temperature). This

inhibition blocks cell division at telophase, thus stopping the proliferation of cancer cells, thus ending its cytotoxic effect. Taxol also promotes the polymerization of tubulin into microtubules, even without GTP, a normally essential cofactor (Bissery, 1991). Thanks to its proven antitumor efficacy, Taxol occupies an essential place in treatment protocols for several types of cancers. In Fig. 6 indicates that the distribution of more than 1200 documents collected from Scopus is over 80% in chemistry, biochemistry, agriculture, pharmacology, medicine, and immunology, among other disciplines, due to the interpenetration of these fields. The most journals of the published articles are summarized in Fig.7.

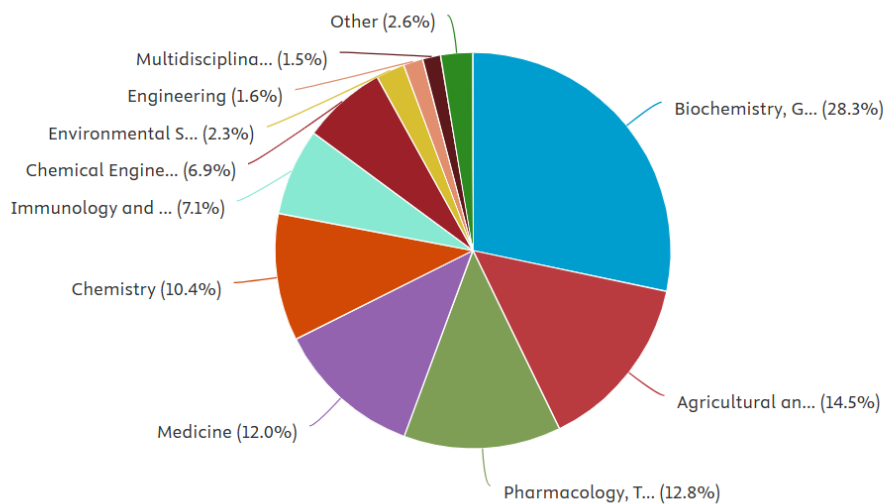


Figure 6: Percentage by domain

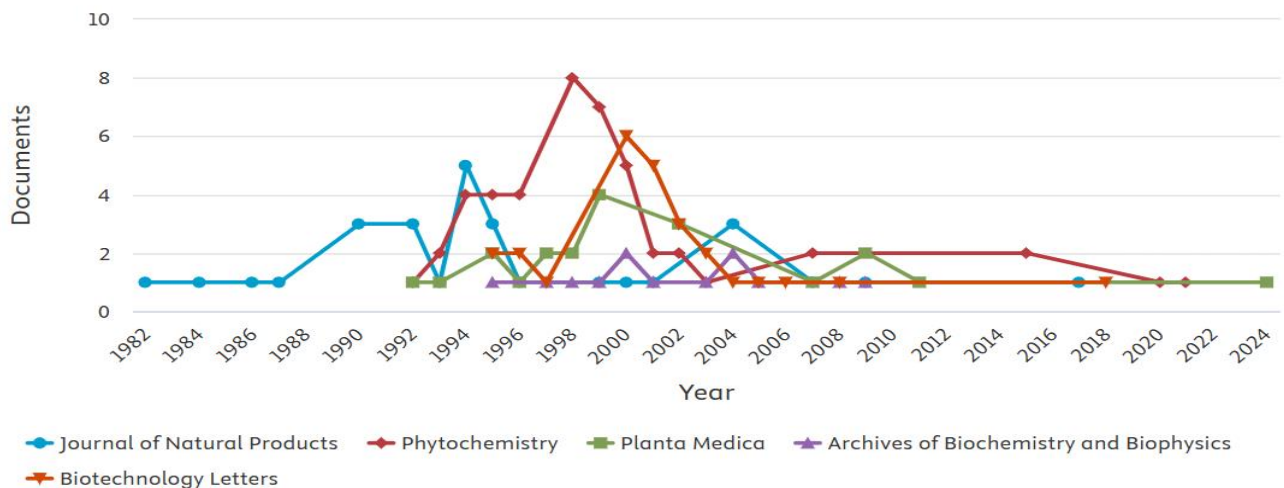


Figure 7: Profiler journals used

The VOSviewer analysis maps authors contributing to Taxol; circles visualize these authors, called “nodes,” in different colors and sizes, depending on the number of articles (Rahaman *et al.*, 2021; Córdoba-Tovar *et al.*, 2022; Hammouti *et al.*, 2025). Among the most highly published authors, there is Croteau from Washington State University, Pullman, US, who has published 37 articles and a total of

309, reaching an IF-index of 95 with more than 28,800 citations across 12,179 documents (Figure 8). The overlay visualization of the most-published authors varies over time, with authors represented in dark purple for articles published before 2000 and yellow for current articles. Figure 9 mentions that Yu and Qiu have more recent publications. The mapping of countries pointed out that China and the US are more interested in the topic due to its importance, followed by India. This bibliometric analysis has been conducted over the last few decades to reorient and rank authors, countries, and collaborations, as shown by lines connecting authors and countries (Figures 8, 9 & 10).

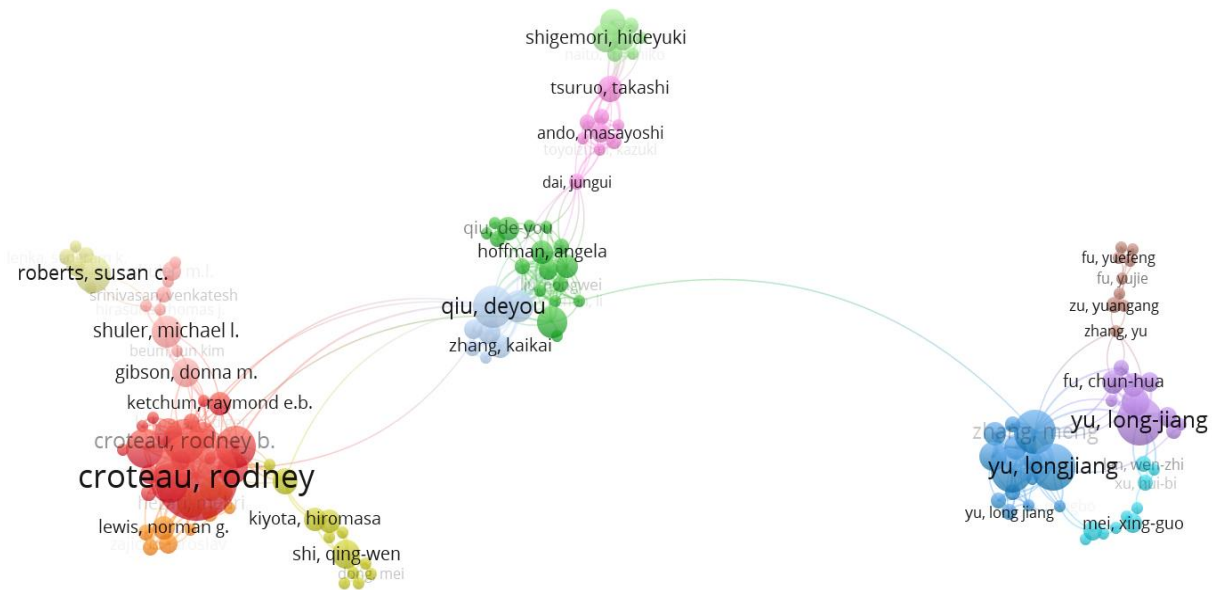


Figure 8: The network visualization of the profiler authors

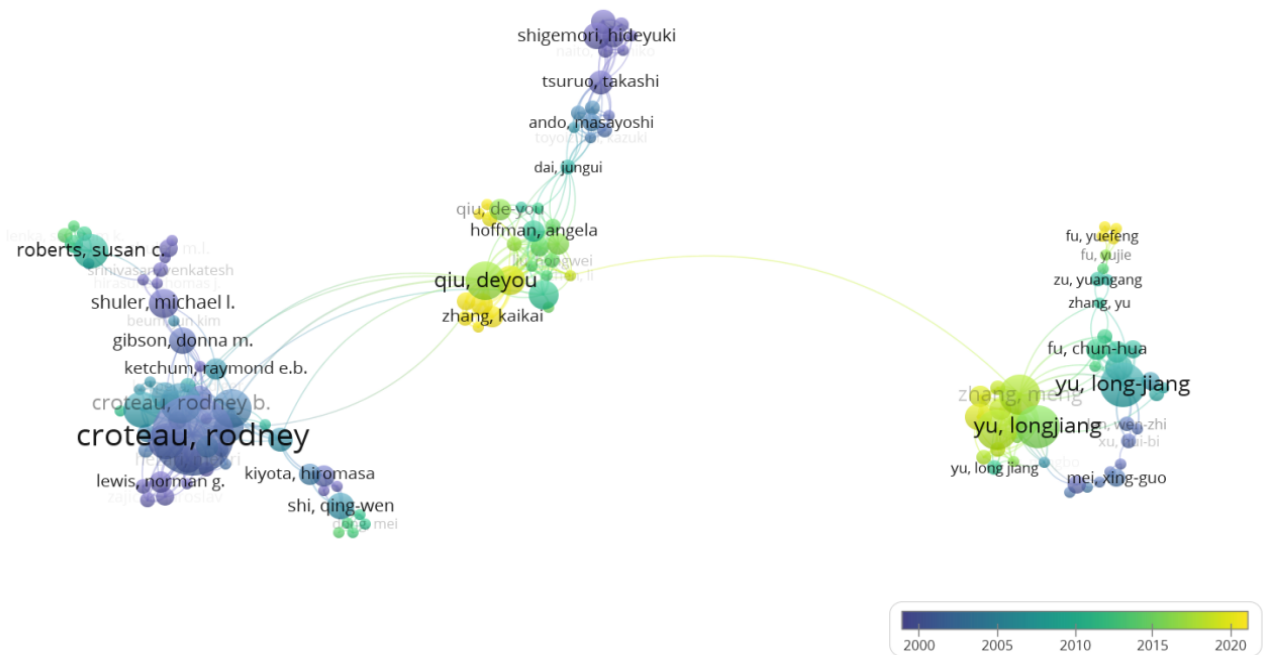


Figure 9: Overlay visualization of the most published authors

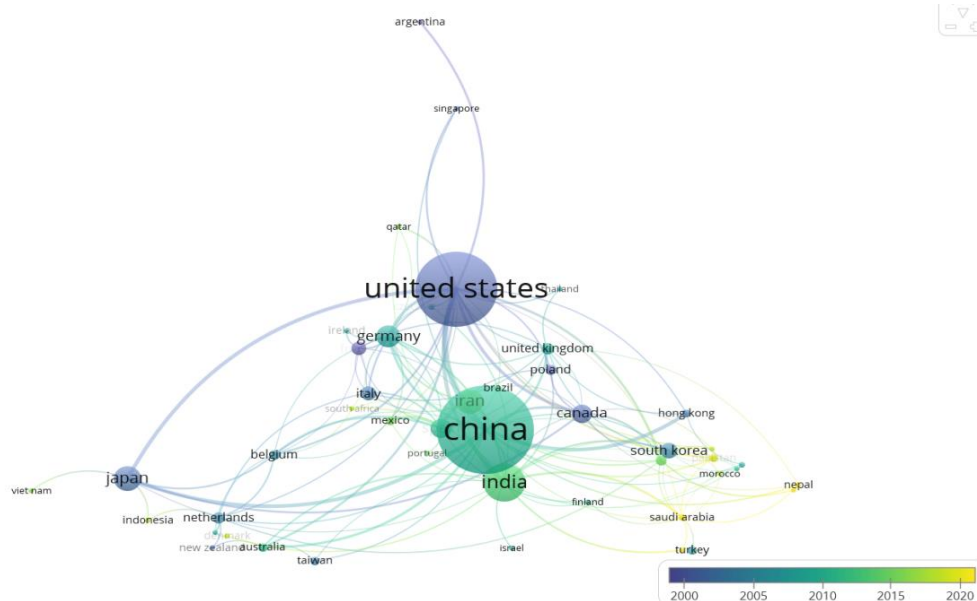


Figure 10: Overlay visualization of the most published countries

8. POM Analysis of Taxol

Taxol, also known as paclitaxel, is a natural antitumor drug derived from the bark of the yew tree (*Taxus spp.*). Its principal bioactivity is its well-known anticancer activity: Taxol is used to treat various types of cancer, including breast, ovarian, and lung cancer. It works by stabilizing microtubules and inhibiting cell division, leading to cancer cell death. It inhibits cell proliferation: Taxol can inhibit cancer cell proliferation by blocking the G2/M phase of the cell cycle. It induces apoptosis: Taxol can induce apoptosis (programmed cell death) in cancer cells, contributing to its anticancer activity.

Taxol is an important drug in the fight against cancer, and it can also have significant antibacterial, antifungal and anti-HIV bioactivities. Taxol (paclitaxel) has been investigated for its potential antiviral activity, particularly in the context of its ability to:

- a. Inhibit viral replication: Some studies suggest that Taxol may inhibit the replication of certain viruses.
- b. Target host cell mechanisms: Taxol's mechanism of action, stabilizing microtubules, may also affect viral replication and transport within host cells.

However, Taxol's primary use remains as the widespread treatment of cancer, whereas its antiviral activity is still being researched. More studies are needed to fully understand its potential as an antiviral agent. Both experimental and theoretical Bioinformatics research are necessary to explore its various pharmacophore sites that are complex combinations to understand, improve its effectiveness and reduce its side effects. Various derivatives of Taxol have been prepared and tested against various biotargets without explaining how to control the selectivity of the new derivatives of Taxol. This is the continuous work one of our favorite topics on natural products ([Brahmi, et al., 2025](#); [Akabli, et al., 2026](#);

Snoussi, et al., 2026; Hamami, et al., 2026; Foufa, et al., 2026). So, POM Theory (Figure 11) was explored for the first time to gain deeper insights into the origin of the multiplicity of these various bioactivities. This natural antitumor, antibacterial, antifungal, and antiviral drug deserves further consideration, as seen below.

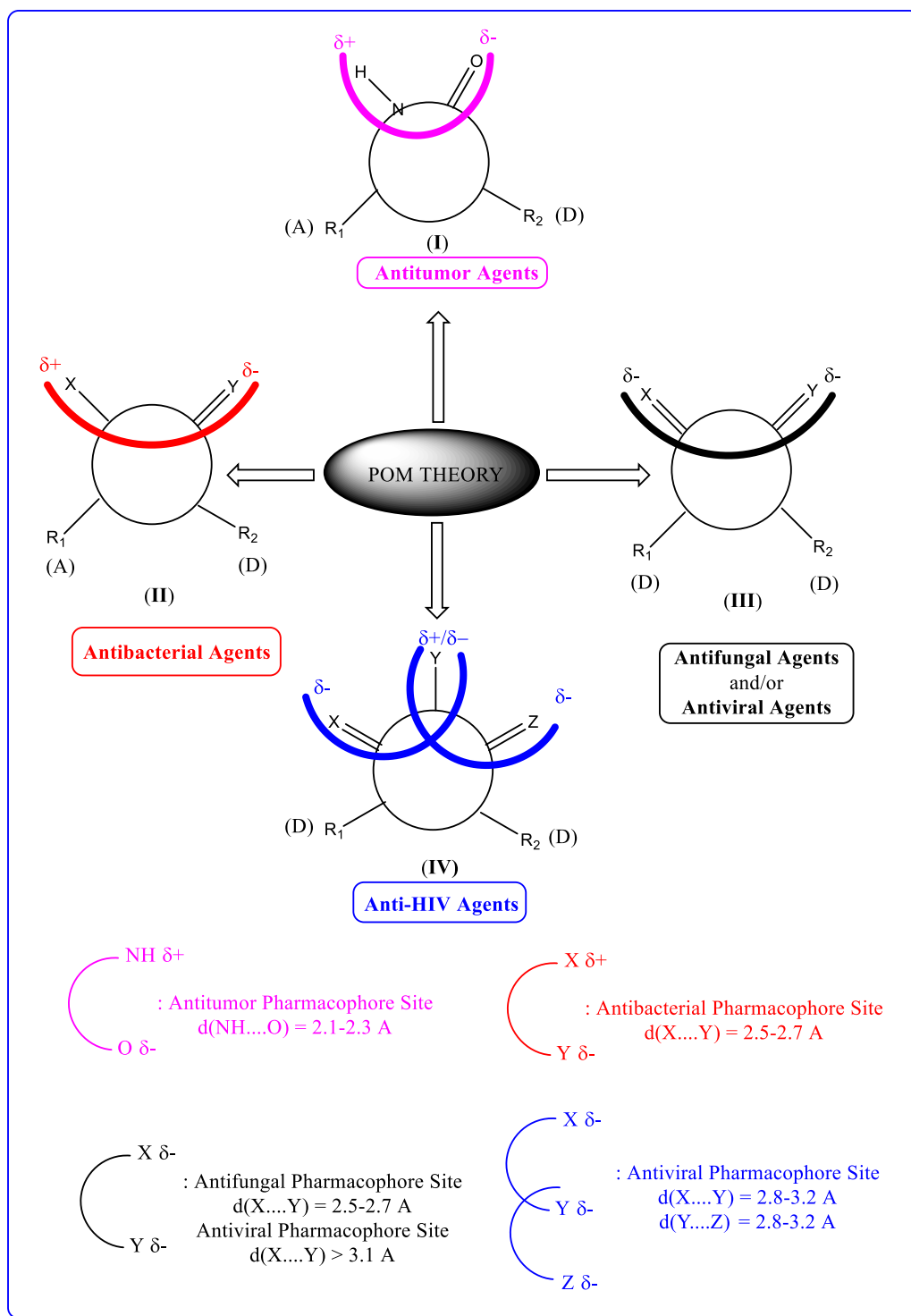
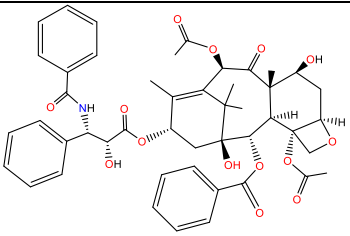


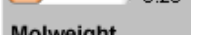

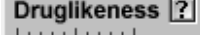
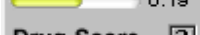
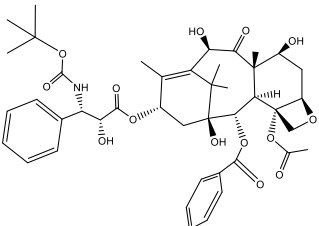






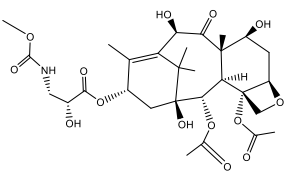




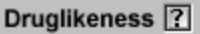
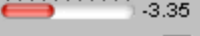
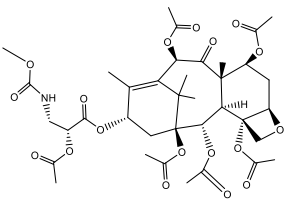








Figure 11: Organigram of POM Theory showing the structure of inhibitors of antibacterial (Rbaa, et al., 2019; Sheikh, et al., 2011 and 2014), antifungal (Titi, et al., 2020), antiviral (Esharkawy, et al., 2022), and antitumor (Bechlem, et al., 2020; biotargets).

Table 1. Calculations of toxicity risks, bioavailability and drug-score of Taxol derivatives.

Compd.	Molecular structure	Toxicity risks	Bioavailability	Drug-score
Taxol		Toxicity Risks <input checked="" type="checkbox"/> mutagenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> tumorigenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> irritant <input type="checkbox"/> ? <input checked="" type="checkbox"/> reproductive effective <input type="checkbox"/> ?	cLogP <input type="checkbox"/> ?  3.19 Solubility <input type="checkbox"/> ?  -6.29 Molweight  853.0	TPSA <input type="checkbox"/> ?  221.2 Druglikeness <input type="checkbox"/> ?  0.19 Drug-Score <input type="checkbox"/> ?  0.22
Docetaxel		Toxicity Risks <input checked="" type="checkbox"/> mutagenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> tumorigenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> irritant <input type="checkbox"/> ? <input checked="" type="checkbox"/> reproductive effective <input type="checkbox"/> ?	cLogP <input type="checkbox"/> ?  2.61 Solubility <input type="checkbox"/> ?  -5.81 Molweight  807.0	TPSA <input type="checkbox"/> ?  224.4 Druglikeness <input type="checkbox"/> ?  -60.4 Drug-Score <input type="checkbox"/> ?  0.16
Hits-1		Toxicity Risks <input checked="" type="checkbox"/> mutagenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> tumorigenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> irritant <input type="checkbox"/> ? <input checked="" type="checkbox"/> reproductive effective <input type="checkbox"/> ?	cLogP <input type="checkbox"/> ?  -1.28 Solubility <input type="checkbox"/> ?  -2.76 Molweight  627.0	TPSA <input type="checkbox"/> ?  224.4 Druglikeness <input type="checkbox"/> ?  -3.35 Drug-Score <input type="checkbox"/> ?  0.29
Hits-2		Toxicity Risks <input checked="" type="checkbox"/> mutagenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> tumorigenic <input type="checkbox"/> ? <input checked="" type="checkbox"/> irritant <input type="checkbox"/> ? <input checked="" type="checkbox"/> reproductive effective <input type="checkbox"/> ?	cLogP <input type="checkbox"/> ?  0.66 Solubility <input type="checkbox"/> ?  -4.4 Molweight  795.0	TPSA <input type="checkbox"/> ?  248.7 Druglikeness <input type="checkbox"/> ?  -3.67 Drug-Score <input type="checkbox"/> ?  0.22

Identification of the Pharmacophore sites of Taxol derivatives

To control the efficiency and selectivity of Taxol derivatives, it is crucial to localize all pharmacophore sites of the parent molecule (Taxol) and then do subtle structural modifications (**Figure 12**). Interestingly, Taxol exhibits a complex combination of different pharmacophore sites that are highly sensitive to the position of the aryl substituents. Certainly, they play an important role in lipophilicity; however, they make the Taxol heavier (MW > 500 g/mole). Docetaxel is the first derivative of Taxol (**Table 1**) and shows a decrease of the Drug-score from 22% to 16%, but the two Hits (noted as 1 and 2) present a better or similar Drug-score than Taxol.

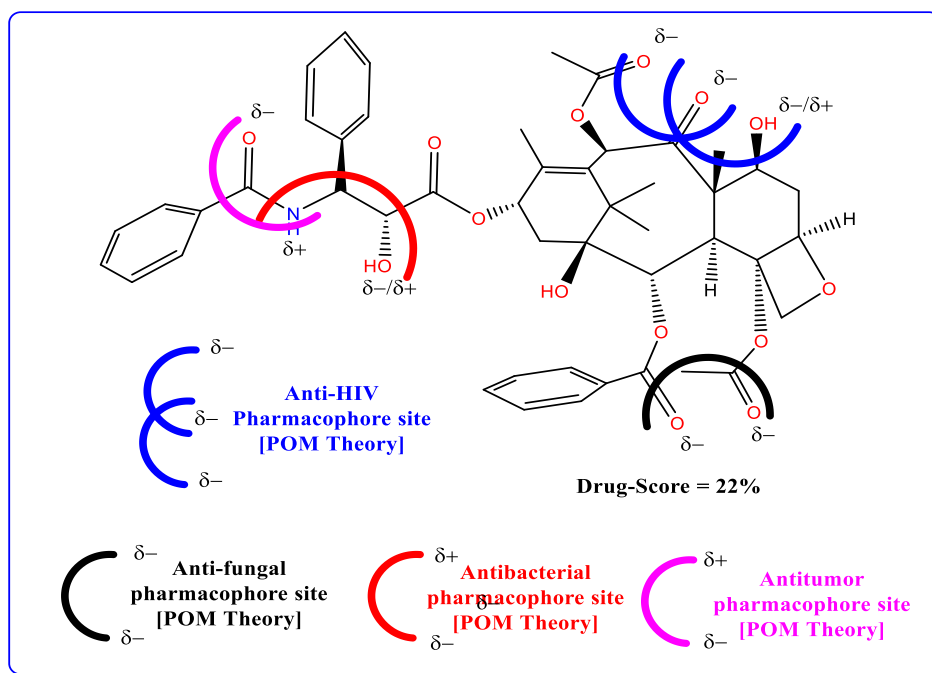


Figure 12: Identification of the pharmacophore sites of Taxol.

9. Conclusion

Taxol (paclitaxel) is one of the most significant and extensively studied anticancer agents oncology. Its complex chemical structure has spurred research into multiple derivatives (such as docetaxel) to optimize its efficacy and bioavailability while reducing its toxicity. Initial extraction techniques based on large-scale harvesting of yew trees posed environmental challenges, leading to the development of complete and semi-synthetic synthesis methods using natural precursors such as 10-deacetylbaccatin III, derived from the European yew (*Taxus baccata*). Taxol and its derivatives have demonstrated notable efficacy in the treatment of various cancers, including breast, ovarian, lung, and Kaposi's sarcoma. To this day, Taxol remains a central component of contemporary chemotherapy and continues to drive research toward developing new, more specific, and less harmful anticancer therapies.

This exceptional journey, from exploration to clinical use, highlights the crucial role of natural substance chemistry and pharmaceutical engineering in the battle against cancer.

Finally, the retrieval of all phenyl groups will lead us to a new derivative (Hits-1) with even more pharmacological performance (Figure 13).

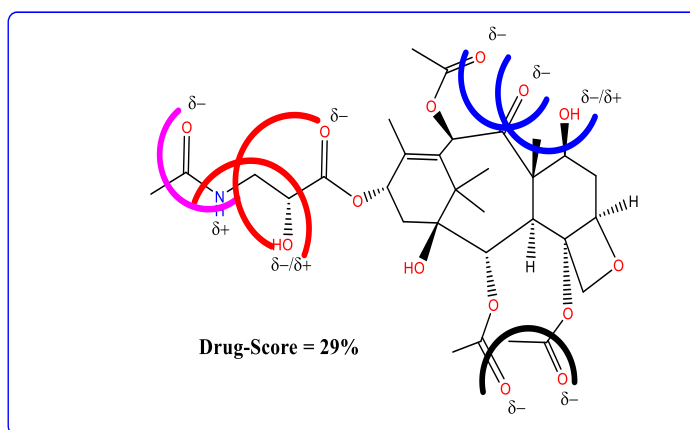


Figure 13: Identification of the pharmacophore sites of Taxol derivative (in perspective).

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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