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# Molecular modeling study of biocides interaction with talc, the main mineral component of soapstone monuments

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CETEM
CENTRO DE TECNOLOGIA MINERAL

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## SUMÁRIO

## RESUMO

Monumentos históricos sofrem, geralmente, de incrustações microbianas. Para evitar isso, muitos produtos químicos são, comercialmente, utilizados como biocidas no tratamento desses patrimônios. Para entender melhor o comportamento físico-químico da interação biocida-talco, a simulação molecular é usada neste trabalho para estudar a interação de três biocidas com o talco, o principal componente mineral dos monumentos da pedra-sabão. As energias de adsorção foram calculadas para definir qual biocida, dentre o timol, etil-p-hidroxibenzoato e o-benzil-clorofenol, se liga melhor à superfície mineral. Os resultados mostraram que os três produtos químicos são adsorvidos, espontaneamente, mas o o-benzil-clorofenol teve a interação mais forte com a superfície mineral. Essa ferramenta computacional se mostrou muito útil e pode ser usada no futuro, não apenas para estudar o melhor agente biocida, mas também para ajudar no design de outros agentes.

**Palavras-chave:**
Modelagem molecular, biocidas, monumentos históricos.

## ABSTRACT

Historical monuments often suffer from microbial incrustation. To prevent that, many chemicals are commercially used as biocides for treating such patrimony. To better understand biocide-talc physicochemical interaction, molecular simulation is used in this work to study the interaction of three biocides with talc, the main mineral component of soapstone monuments. Adsorption energies were calculated in order to define which biocide out of thymol, ethyl-p-hidroxybenzoate and o-benzyl-chlorophenol better binds to the mineral surface. Results showed that all three chemicals are spontaneously adsorbed, but o-benzyl-chlorophenol had the strongest interaction with the mineral surface. This computational tool proved very useful and can be used in the future, not only to study the best biocide agent, but also to help in design other agents.

**Keywords**:
Molecular modeling, biocides, soapstone monuments.

# 1 | INTRODUCTION

## 1.1 | Biodeterioration

The growing concern with the preservation of the monuments that are part of the historical and cultural patrimony has led to a greater interest in the biodeterioration of these constructions (WARSCHEID & BRAAMS, 2000), since they are structures susceptible to degradation caused by microorganisms sticked to their surface (CRISPIM, 2003).

Historical monuments undergo a natural wearing process caused by environmental conditions, leading to substantial material losses. This wearing phenomena are caused by wind, rain, air pollution, chemical and biological factors, that include fungi, bacteria, cyanobacteria, algae and lichens (ALVES, 2012). The growth of microorganisms compromises the performance of materials, their aesthetic appearance and may present a health risk (ERICH & BAUKH, 2016). Monitoring the bio- deterioration process with minimal impact on the work of art and environment is a challenge for professionals in the area of preservation (LOPES et al., 2003).

The biodeterioration of stone materials rarely occurs by the presence of only one group of organisms; different species of microorganisms may coexist. During the life cycle, these microorganisms interact with the stone, which can lead to deterioration of the monuments. In this way, they bring about combined changes in monuments through the products of their metabolism (PRADO et al., 2009).

One of the most complex problems of conservation of monuments is the biological knowledge and little information in the area regarding the biodeterioration. Thus, techniques

of microbiology associated with molecular analysis represent a new perspective of studies in advanced researches for conservation of historical patrimony (MILLER et al., 2008).

Biodeterioration occurs with the formation of biofilms on the affected substrate. Biofilms are complex biological systems made up of several taxonomic and metabolic groups of microorganisms that are associated with the surface or intrinsic, invading, in some cases, the major part of buildings (MORALES & DUQUE 1998; SANTOS, 2011). Thus, the search for new subsidies for the preservation of this patrimony becomes imperative (RESENDE, 2002).

The development of new biocides is important for those in charge of conservation rocky materials. However, most biocides, commonly used, were developed for agronomic purposes and, therefore, not specifically designed for using in restoration of artifacts of historical value. In these cases, interactions with different substrates must be carefully tested to avoid undesirable modifications (KOESTLER & SALVADORI, 1996).

## 1.2 | Soapstone Monuments

Historical cities traditionally seek for keeping their heritage alive and preserved, usually in the form of monuments that are part of the history of a certain place, country or even in some cases standing out as a patrimony of humanity. In the specific case of the city of Ouro Preto, located in the state of Minas Gerais, Brazil, its monuments are largely constituted of the mineral steatite (*i.e.*, by mass, "pure" steatite is roughly 63.37% silica, 31.88% magnesia, and 4.74% water. It commonly contains minor quantities of other oxides such as CaO or

$Al_2O_3$), or soapstone, names used for a metamorphic rock whose origin is in physical and chemical processes that occur in a particular mineral mass, composed mainly of talc, but also containing in its composition other minerals, such as magnesite, chlorite, tremolite and quartz, among others.

Soapstone is a rock that presents very soft and low hardness, due to its possessing in its constitution with large amounts of talc, can be found in several colors ranging from gray to green. In Ouro Preto there is a great number of people who live from manufacturing sculptures in soapstone. In this art, the craftsman Antônio Francisco Lisboa, Aleijadinho (1738-1814), who surpassed all the physical limitations imposed by a "mysterious disease", which took him from 1777, created hundreds of sculptures that are still available today for visitation, as well as adornments in churches and facades, one of them is the Church of São Francisco de Assis (Figure 1).

Source: Wikipedia.

**Figure 1**. Facade of the Church of São Francisco de Assis in Ouro Preto.

Even with all this, the discovery of soapstone did not occur in Ouro Preto, since it was already used before Christ in the Middle East. Over the centuries, the discovery of its characteristics made it used in many European fireplaces and sculptures in Asia Minor. It is a very sturdy rock. that is why we find it in Cristo Redentor monument, in the city of Rio de Janeiro. But even with this resistance, time is relentless with these monuments. Whether by climatic means, biological or by predatory human action, these monuments invariably need a restoration in their structures over time.

CETEM (Centre for Mineral Technology) has experience in restoration studies in several brazilian historical monuments (QUEIROZ & RIBEIRO, 2015; SANTOS & RIBEIRO, 2015; DALTO & RIBEIRO, 2016; MOURA & RIBEIRO, 2017; BARBUTTI & RIBEIRO, 2017; BARBUTTI & RIBEIRO, 2018; TASCA et al., 2018). Following that line of research, this work provides one more contribution by using computational modeling techniques. Figure 2 illustrates this line of thought.

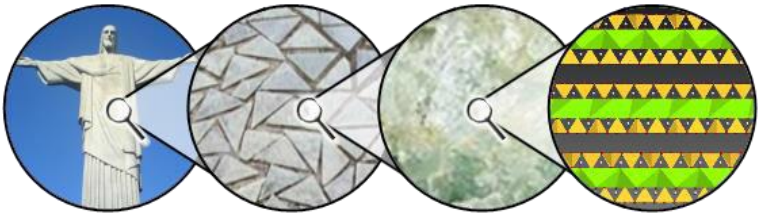

**Figure 2**. Multiscale look into a monument's structure.

## 1.3 | Adsorption of Organics on Minerals

Adsorption phenomena regard the deposition of species such as ions or molecules into a surface by physical or chemical

interactions. The frontier between physical and chemical adsorption is not always clear, with the usual energy limits not being constant for different kinds of systems. Asaduzzaman et al. (2014) studied adsorption of organic molecules on mineral surfaces and were able to define regions of weak, intermediate and strong adsorption based on the adsorption energies of single molecules: from 0 to 0.5 eV/mol, mostly physisorption; from 0.5 to 1 eV/mol, molecules are moderately polarized; and from 1 eV/mol onward, chemisorption, ionic bonding or strong polarization take place.

## 1.4 | Molecular Modeling

Molecular Modeling comprises many families of computational techniques by which it is possible to study the properties of matter at atomic level. Molecular Mechanics makes use of energy expressions called force fields to treat molecular systems by means of classical mechanics equations. Atoms are treated as particles with mass, charge and other specific parameters, while chemical bonds are treated as springs connecting two atoms. The extensive work of many researchers throughout the last decades has made molecular mechanics an exceptional tool for computational studies of chemical systems. Some important concepts are reviewed ahead.

### 1.4.1 | Energy minimization

Energy Minimization applies an optimization algorithm on a system of particles to minimize its total potential energy by iteratively adjusting the values of relative distances, bond

lengths, and other geometric variables. It's almost mandatory in any molecular mechanics calculation. It is also called Geometry Optimization.

### 1.4.2 | Molecular dynamics

Molecular dynamics (MD) is the term used to describe the solution of the classical equations of motion (Newton's equations) for a set of molecules (ALLEN & TILDESLEY, 2017). Newton's equations of motion are numerically integrated in small time steps and the interaction forces between particles are computed. A statistical ensemble is defined, in which three quantities will be kept constant during the simulation, the most common being the Canonical or NVT ensemble (constant number of particles, volume and temperature), the Isothermal–Isobaric or NPT ensemble (constant number of particles, pressure and temperature) and the Microcanonical or NVE ensemble (constant number of particles, volume and total energy). The microscopic mechanical quantities are related to the macroscopic thermodynamic quantities by statistical thermodynamics.

### 1.4.3 | Quenching and simulated annealing

Quenching is a combined Molecular Dynamics and Geometry Optimization approach. A regular molecular dynamics run is started and, every given number of steps, the structure of the system has its energy minimized and saved in a separate trajectory (O'CONNOR et al., 1991). By doing that, conformational space can be efficiently sampled.

Simulated Annealing (KIRKPATRICK et al., 1983), on the other hand, simulates the cooling of a system from high temperature. It can be used as a protocol consisting of cycles of heating and cooling during a molecular dynamics run. These cycles through different temperatures enable the system to reach energy states it could otherwise not, mostly because of local energy minima. It can be combined with the Quenching approach, leading to a very efficient method to scan the conformational space and find stable low energy conformations for molecules and systems.

## 2 | OBJECTIVES

This work aims at using molecular simulation as a tool to evaluate the interaction of three biocides used in conservation with the talc mineral, main component of soapstone. Thymol (2-isopropyl-5-methylphenol), Asseptin A (ethyl-p-hydroxybenzoate) and Preventol BP (o-benzyl-p-chlorophenol) were selected for this study and are shown in Figure 3.

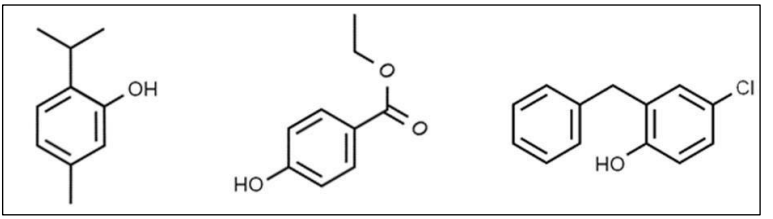


**Figure 3**. Representations of thymol, ethyl-p-hidroxybenzoate and o-benzyl-chlorophenol, respectively.

## 3 | METHODOLOGY

The defined methodology comprised three major parts:

- Biocides modeling and conformational analysis;
- Talc modeling, optimization and surface construction;
- Talc-biocide systems construction, simulation, and adsorption energies calculation.

The Consistency Valence Force Field (CVFF) (DAUBER-OSGUTHORP et al., 1988) is widely used to model organic molecules' atomic potentials and was chosen to model the biocide molecules, while the parameters from its augmented ionic version, CVFF_aug (HILL et al., 2000) were used to model the mineral.

### 3.1 | Biocides Modeling

Each biocide molecule was constructed and had its geometry optimized. Then they went through a conformational search by means of Quenched Simulated Annealing procedure, consisting of 10 cycles, from 1 $^{o}$K to 500 $^{o}$K, during 1 ns dynamics run with time steps of 1fs. Structures were quenched at the end of every cycle.

After obtaining the low energy conformers, those with the lowest potential energy underwent 1 ns of NVT molecular dynamics at 298 $^{o}$K in vacuum. The last half of the trajectory was analyzed to obtain the average potential energy. This procedure is due to the thermalization instability that always occurs in the beginning of dynamics runs.

## 3.2 | Talc Mineral Modeling

Talc crystal unit cell structure file was imported from a crystallographic database and it is based on the reports of Grunner (1934). The original cell did not have the hydrogen atoms of the hydroxyls corresponding to the natural hydration state of this mineral, so they were added. The unit cell then went through geometry optimization. Talc surface was created from its unit cell, which was multiplied into a supercell, and then cleaved between its sheets, exposing talc's basal plane. A 10 nm vacuum layer was added on top of it. Figure 4 illustrates this process.

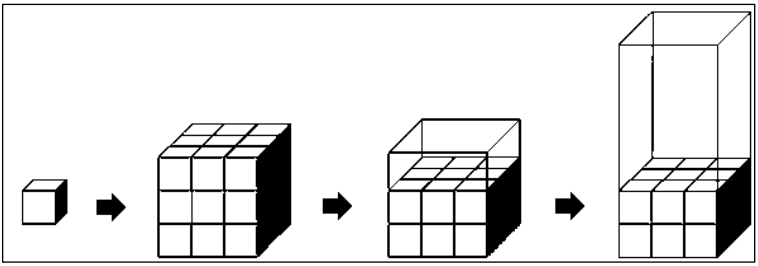

**Figure 4**. Surface construction: unit cell, supercell, cleaved surface and surface in vacuum, respectively.

## 3.3 | Biocides on Talc Surface

The lowest energy conformer of each biocide molecule was separately put in contact with the talc surface. Molecular dynamics of 200 psi NVT ensemble at 298 $^{o}$K were run and the last half of the trajectories were used to calculate the average potential energy of the system. As a conformational analysis step, the ten structures with lower potential energy were selected from the trajectory and optimized.

To investigate which biocide better interacts with the mineral, adsorption energies ($E_{ads}$) were calculated for each molecule. The lower the energy, the better the interaction of the molecule with the mineral substrate. Equation 1 shows how this energy is calculated:

$$E_{ads} = E_{system} - (E_{biocide} - E_{mineral}) \quad [1]$$

where $E_{system}$ = potential energy of the system biocide-mineral in contact; $E_{biocide}$ = potential energy of biocide molecule alone in vacuum; and $E_{mineral}$ = potential energy of the mineral surface in vacuum (considered zero for calculations purpose). $E_{ads}$ was computed in two ways:

- Using the average potential energies of the systems from their dynamics runs at 298 $^{o}$K;
- Using the lowest optimized potential energies obtained from conformational analysis.

Results were than compared.

## 4 | RESULTS AND DISCUSSION

### 4.1 | Biocides Modeling

The quenched annealing resulted in 10 minimized structures for each biocide. Their conformations and potential energy x frequency plots are shown in Figure 5.

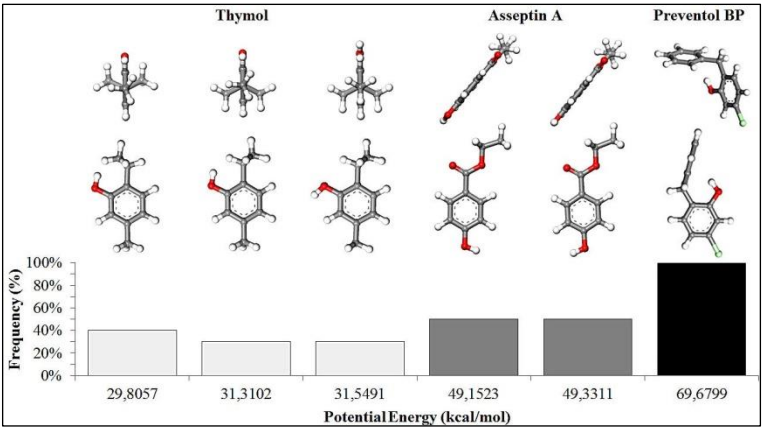


**Figure 5**. Biocides conformations, energy and frequency.

Thymol's annealing resulted in three conformers with close frequency. The lowest energy one appeared in 4 out of the 10 structures, while the other two appeared three times each. It is possible to note that the difference in conformation is due to three specific movements: the rotation of the methyl group around the C-C bond's axis, the rotation of the hydroxyl group around the C-O bond's axis and the isopropyl group rotation around the C-C bond's axis.

Asseptin A's results show two conformers with same frequency and very close energy. That is because the only difference between them is the rotation of the hydroxyl group. As expected, being an aromatic ring linked to ester, its stable structure is planar. Preventol BP showed only one conformer in all the ten structures. Its central carbon has tetrahedral geometry and the two aromatic rings are perpendicular to each other. The energies obtained throughout all the methods applied to the biocides are summarized in Table 1.

**Table 1**. Potential energies obtained throughout the biocides modeling.

| | Potencial Energy (Kcal/mol) | | |
|---|---|---|---|
| **Molecule** | **First Optimization** | **Quenched** | **Dynamics average** |
| Thymol | 30,5224 | 29,8057 | 48,3540 |
| Asseptin A | 49,7179 | 49,1523 | 61,6710 |
| Preventol BP | 71,7861 | 69,6799 | 89,3610 |

As expected, average potential energies from the dynamics runs are higher than the optimized and quenched ones. That is because of the kinetic energy, which keeps atoms in motion, prevents the molecules from reaching lower potential energy states.

## 4.2 | Talc Mineral Modelling

The talc united cell, imported from the database, went through optimization, resulting in the following parameters given in Table 2.

**Table 2**. Talc unit cell parameters before and after optimization.

| | Lenghts (Å) | | | Angles (°) | | |
|---|---|---|---|---|---|---|
| Unit cell | a | b | c | α | β | γ |
| Before optimizing | 5,260 | 9,100 | 18,810 | 90,00 | 100,00 | 90,00 |
| After optimizing | 5,296 | 9,103 | 18,215 | 90,00 | 101,99 | 90,00 |

The original cell parameters are experimental values, and the optimized cell parameters are derived from the force field calculation. The values from before and after optimization are in good agreement, what proves the ability of the used force field in describing the structure of talc. Figure 6 shows talc optimized structure.

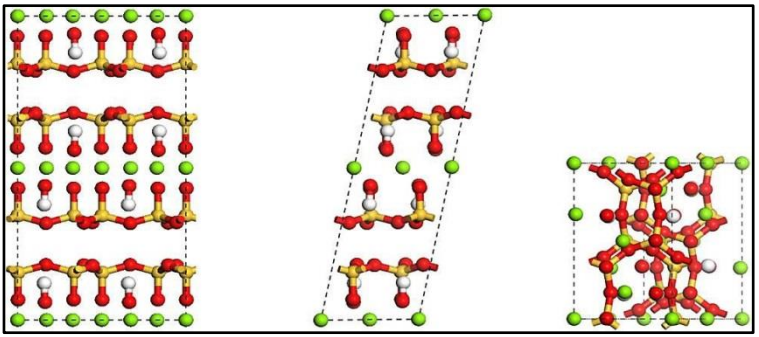

**Figure 6**. Talc optimized unit cell: frontal, lateral and superior views, respectively.

## 4.3 | Biocides on Talc Surface

Ten optimized structures were obtained after the dynamics runs of the talc-biocide systems. The less energetic structure of each system, its frequency among the ten structures and the standard deviation of the sample are summarized in Table 3.

**Table 3**. Results from the biocide-talc systems' dynamics and optimization.

| Molecule | Lowest Potential Energy (Kcal/mol) | Frequency (%) | Standard Deviation |
|---|---|---|---|
| Thymol | 12,5672 | 30,0 | 1,3420 |
| Asseptin A | 27,5682 | 30,0 | 0,4737 |
| Preventol BP | 48,7929 | 20,0 | 0,5822 |

The Eads values were calculated from the potential energies reported in Table 3 and from the average potential energies obtained in the dynamics runs. The results are presented in Table 4.

**Table 4**. Energy of adsorption calculated for each system.

| Energy of adsorption (Kcal/mol) | | |
|---|---|---|
| Molecule | Optimized system | Dynamic average |
| Thymol | - 17,2384 | - 12,5192 |
| Asseptin A | - 20,6422 | - 14,2130 |
| Preventol BP | - 20,8870 | - 16,7350 |

All three biocides showed negative $E_{ads}$, which means spontaneous adsorption process. All results are within the intermediate region of adsorption strenght (Asaduzzaman *et al*. 2014), which indicate stronger than usual, but still physical adsorption. Given the fact that the studied molecules were all almost water-insoluble organic compounds, these results agree well not only with the known chemical stability but also with the inherent hydrophobicity of talc's basal planes, due to its silicate sheets without exposed ions or hydroxyl groups (CHABROL et al., 2010).

The values of $E_{ads}$ calculated by both methods show the same trend, putting Thymol, Asseptin A and Preventol BP in ascending order of stability, that indicates that Preventol BP is the best adsorbate for talc basal surface; although, all the three biocides showed adsorption energies in the intermediate region, with a maximum difference of 4,2158 kcal/mol between Preventol and Thymol. It should be noted that Preventol had the worst optimization gain from dynamics. That is probably due to the natural perpendicular arrangement of its two aromatic rings, preventing it from adjusting more efficiently to the talc plane. Asseptin A, on the other hand, had the best gain with the optimization, probably due to its naturally planar structure. In the case of Thymol, its isopropyl tail also prevents its aromatic ring from perfectly adjusting to the mineral planar surface. Figure 7 shows the structures of the optimized systems whose energies are reported in Table 6.

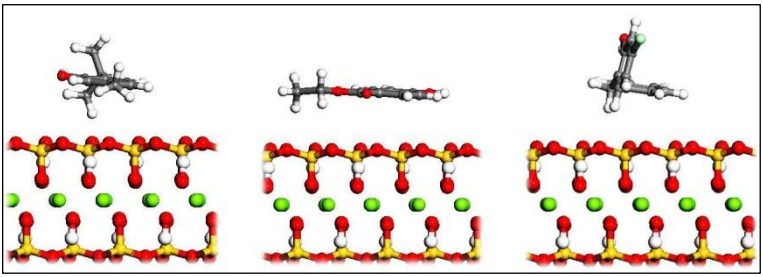

**Figure 7**. Best conformations of biocides on talc: Thymol, Asseptin A and Preventol BP, respectively.

## 5 | CONCLUSIONS

Molecular simulation techniques were used to study the adsorptive behavior of Thymol, Asseptin A and Preventol BP on talc surface. The values found for adsorption energies were in agreement with strong physisorption range of values, what relates well with talc's basal planes inherent chemical stability. Although all three biocides showed spontaneous adsorption (negative $E_{ads}$), Preventol BP was the one with the most favorable energetics, indicating that it binds better to the mineral surface, and as such, is less prone to be removed from it by weathering, for example.

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