



Acelerando a Descoberta de Novos Fármacos com Qt

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Qt

1. Introdução

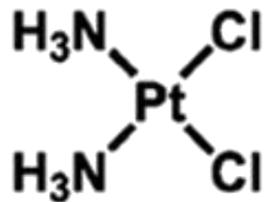


COMPOSTOS BASEADOS EM PLATINA

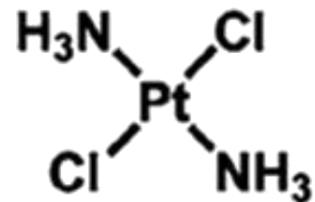
Um exemplo é a cisplatina, que é um fármaco utilizado na maioria dos protocolos de tratamento de diversos tipos de câncer, tais como: testículos, ovários, garganta, bexiga, esôfago, dentre outros.

 Qt

COMPOSTOS BASEADOS EM PLATINA



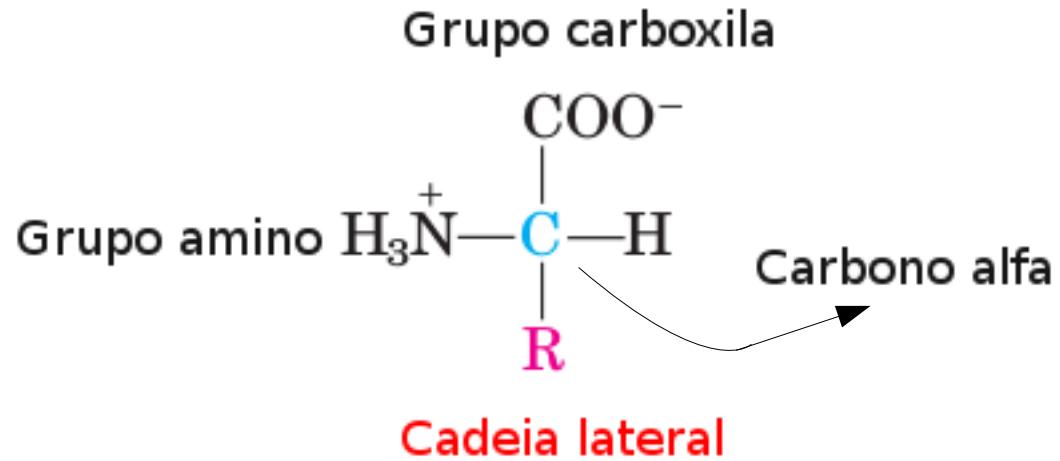
Cisplatina



Transplatina

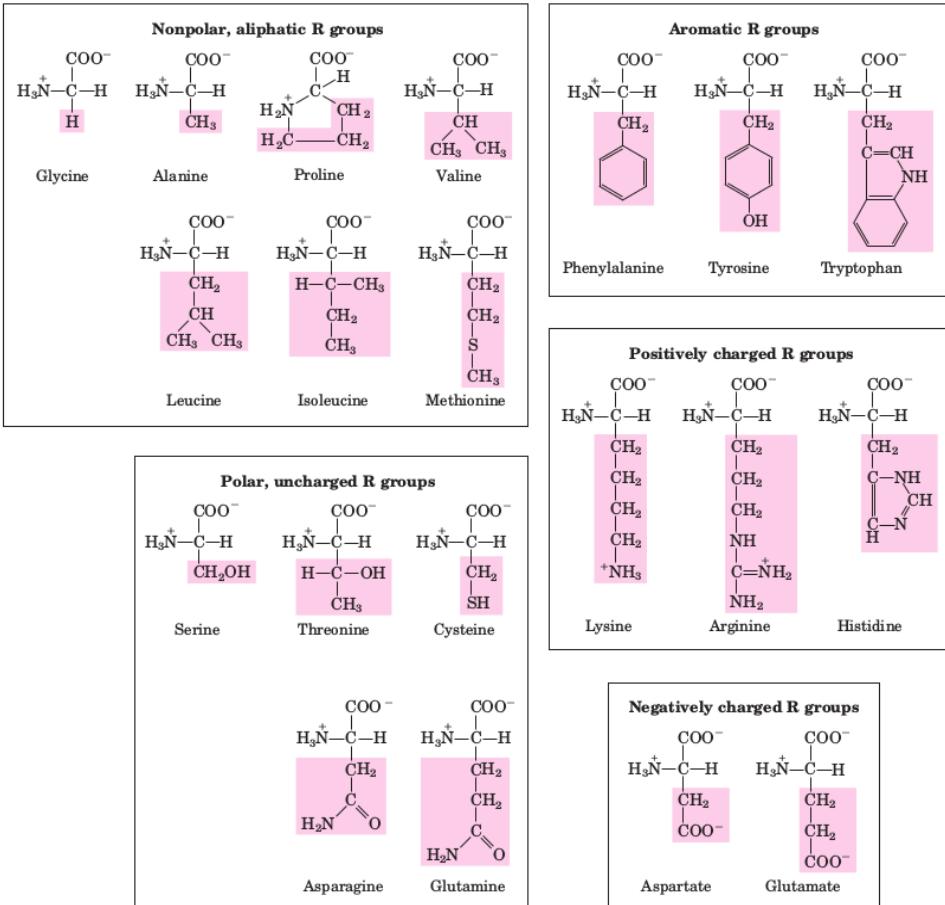
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AMINOÁCIDO



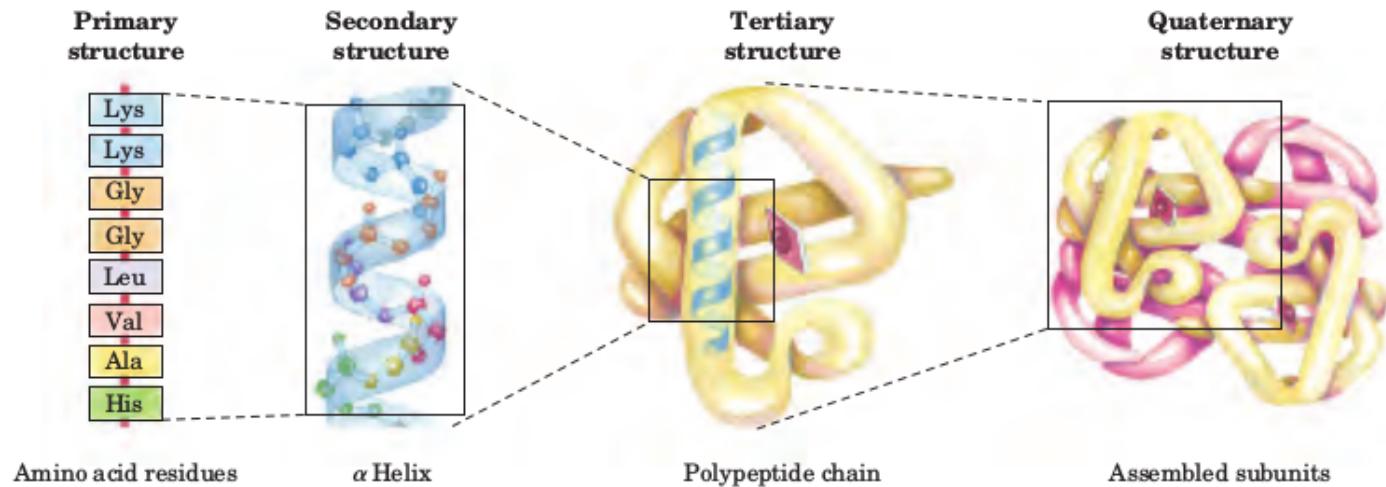
Qt

20 TIPOS DE AMINOÁCIDOS



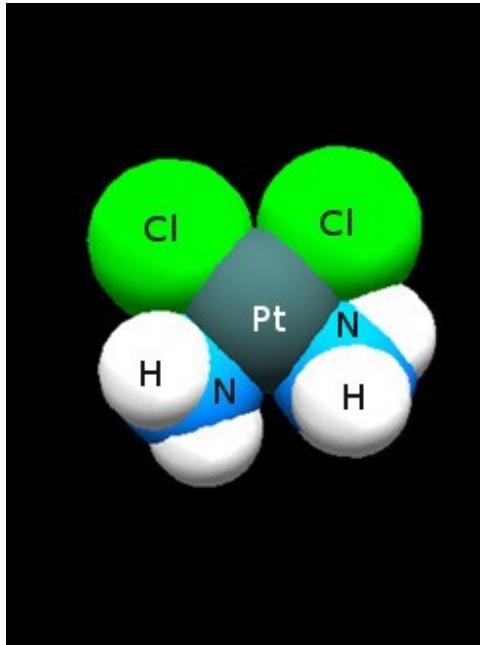
Qt

ESTRUTURAS DAS PROTEÍNAS

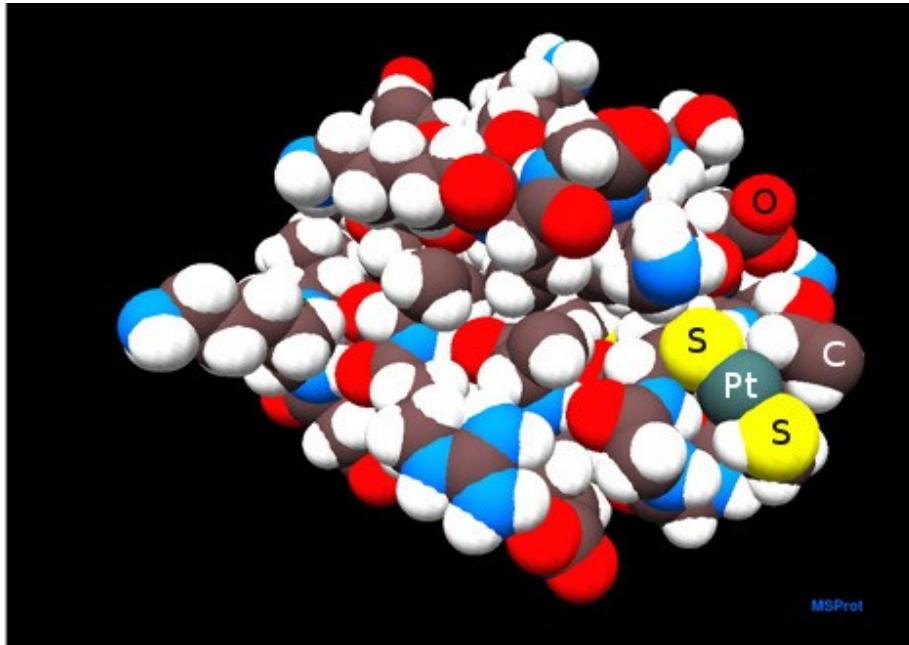


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CISPLATINA



CISPLATINA ACOPLADA A PROTEÍNA



Qt

Imagens geradas pelo software MSProt.

CISPLATINA ACOPLADA A PROTEÍNA

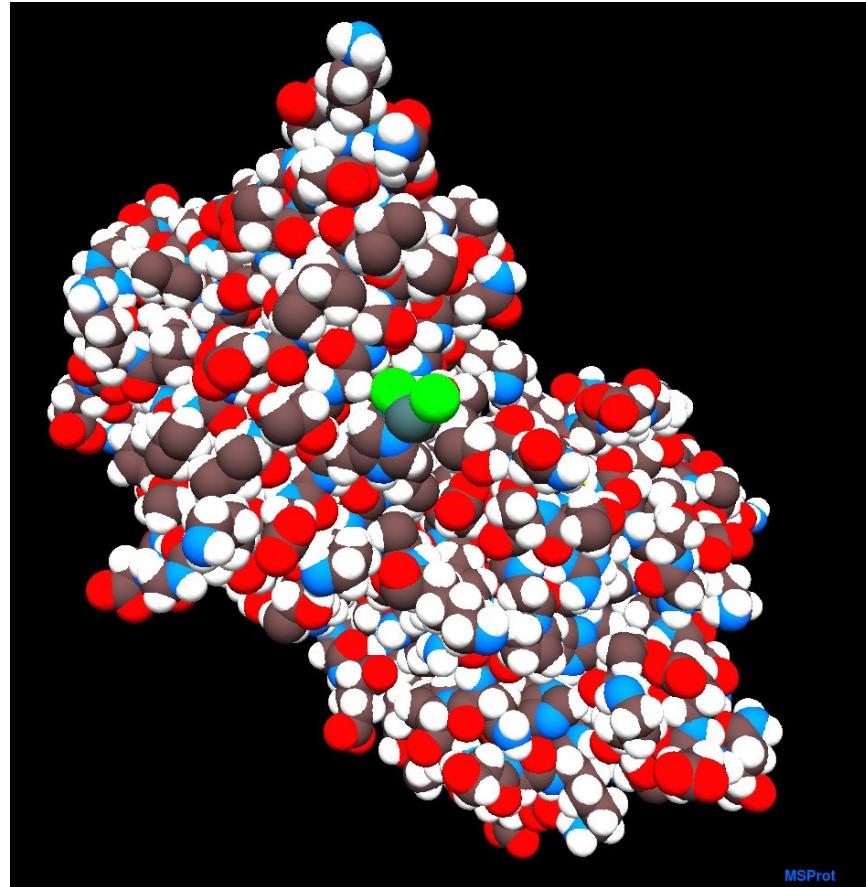


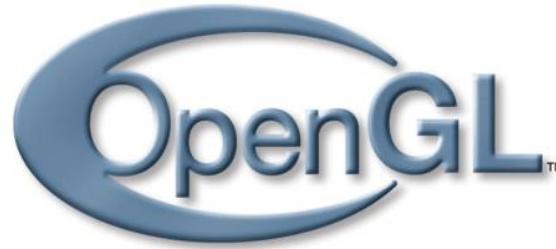
Imagen geradas pelo software **MSProt**.

2. Materiais e Métodos

Qt



PLATAFORMA DE DESENVOLVIMENTO

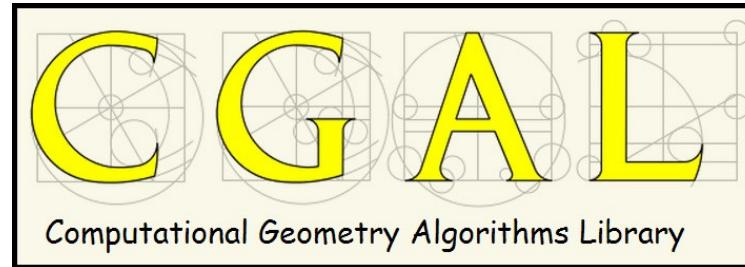


Versão 5.3.1 (LINUX)

PLATAFORMA DE DESENVOLVIMENTO



Versão 5.0



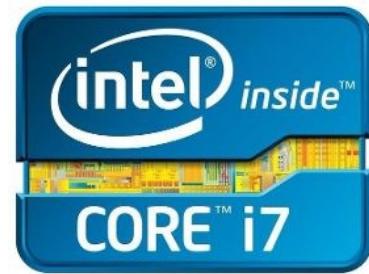
Versão 4.4

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HARDWARE



Nvidia Titan Black 6 Gb de memória
384-bit GDDR5, 2880 núcleos



Processador Core i7 3,80 GHz
Cache de 8M, 4 núcleos e 8 threads

32Gb de memória RAM DDR2

Qt

FUNÇÕES VIRTUAIS

```
class MyGLDrawer : public QGLWidget
{
    Q_OBJECT           // must include this if you use Qt signals/slots

public:
    MyGLDrawer(QWidget *parent)
        : QGLWidget(parent) {}

protected:
    void initializeGL()
    {
        // Set up the rendering context, define display lists etc.:
        ...
        glClearColor(0.0, 0.0, 0.0, 0.0);
        glEnable(GL_DEPTH_TEST);
        ...

    }

    void resizeGL(int w, int h)
    {
        // setup viewport, projection etc.:
        glViewport(0, 0, (GLint)w, (GLint)h);
        ...
        glFrustum(...);
        ...

    }

    void paintGL()
    {
        // draw the scene:
        ...
        glRotatef(...);
        glMaterialfv(...);
        glBegin(GL_QUADS);
        glVertex3f(...);
        glVertex3f(...);
        ...
        glEnd();
        ...
    }
};
```

initializeGL() - Responsável pelo contexto do OpenGL. Define, por exemplo, tipo de luz e material.

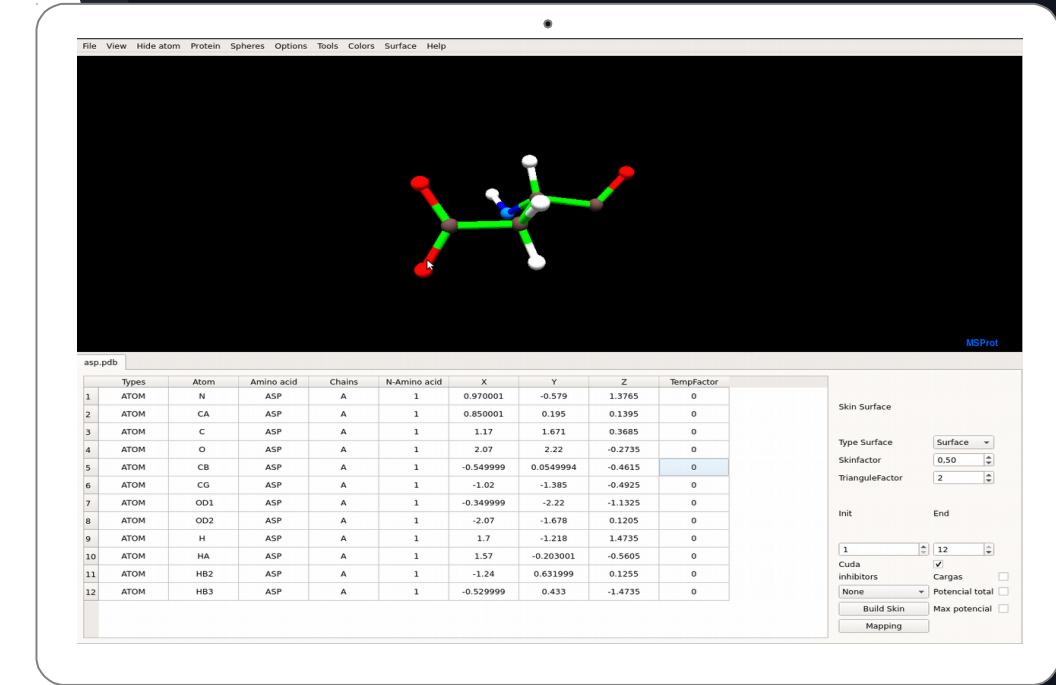
resizeGL() - Define, por exemplo, o viewport e a matriz de projeção.

paintGL() - Renderiza a cena.

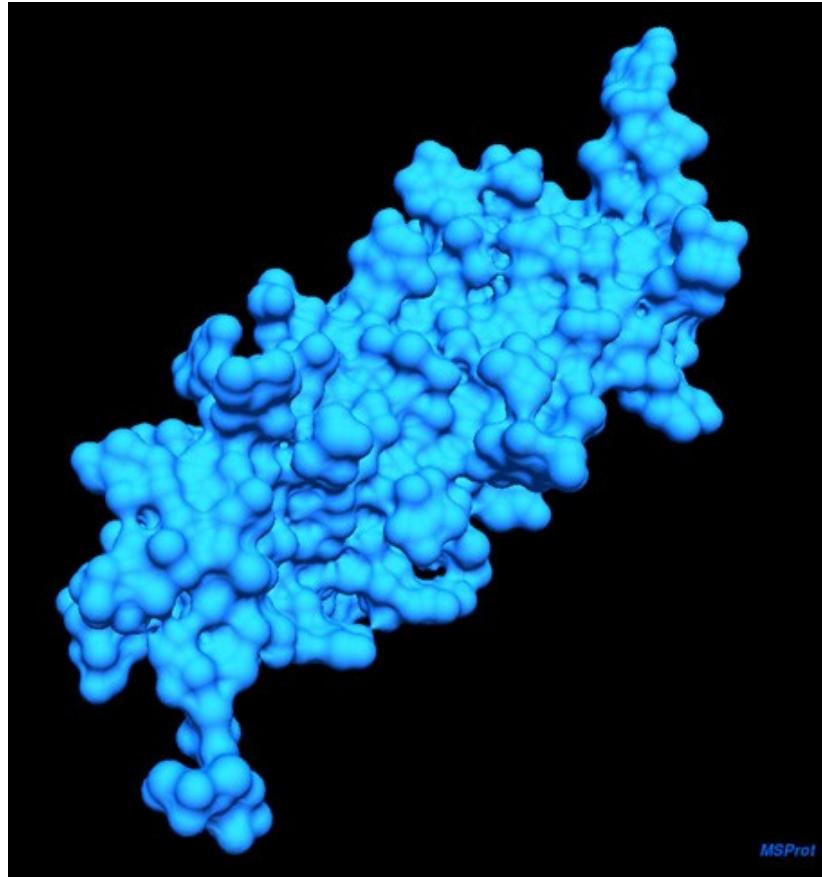
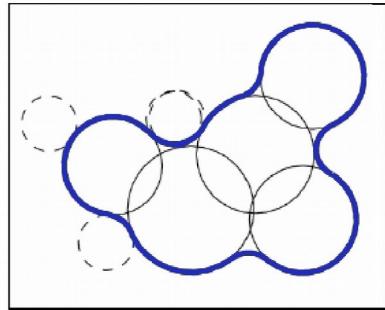
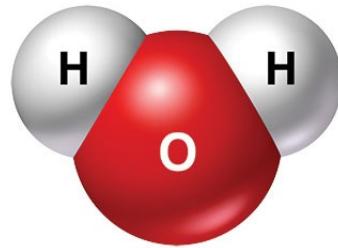
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MSProt em ação!!!



SUPERFÍCIE MOLECULAR (SKIN SURFACE)



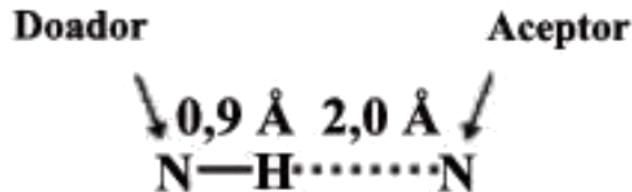
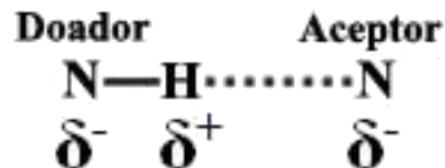
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LIGAÇÕES DE HIDROGÊNIO

Aceptor - Aceita um próton de hidrogênio



Doador - Doa um próton de hidrogênio



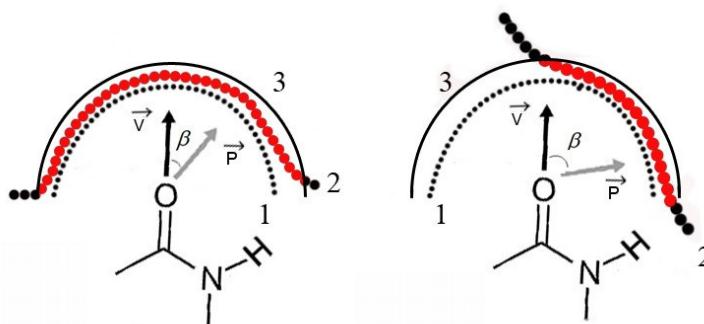
$$1 \text{ \AA} = 10^{-10} \text{ m}$$

MAPEAMENTO DA SUPERFÍCIE MOLECULAR

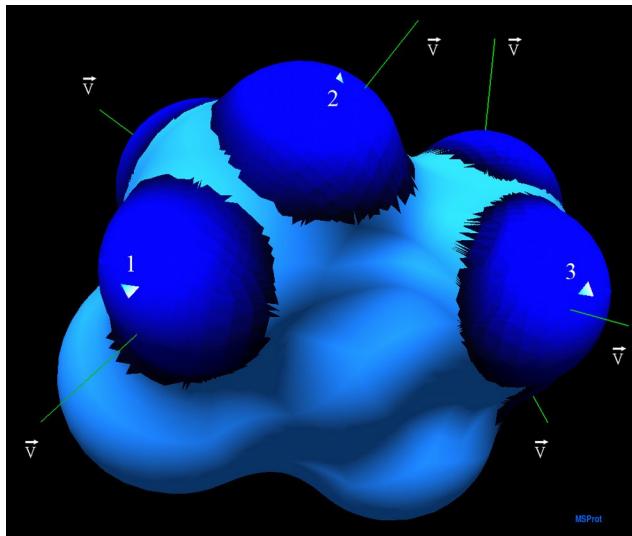
Aceptor - Aceita um próton de hidrogênio



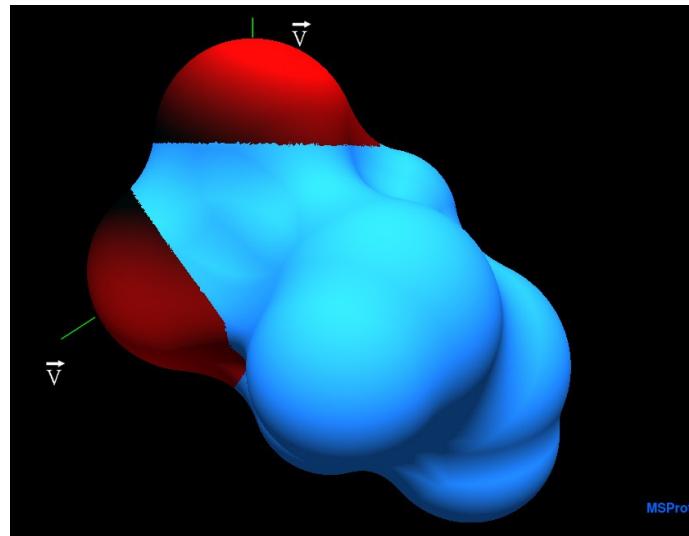
Doador - Doa um próton de hidrogênio



CISPLATINA

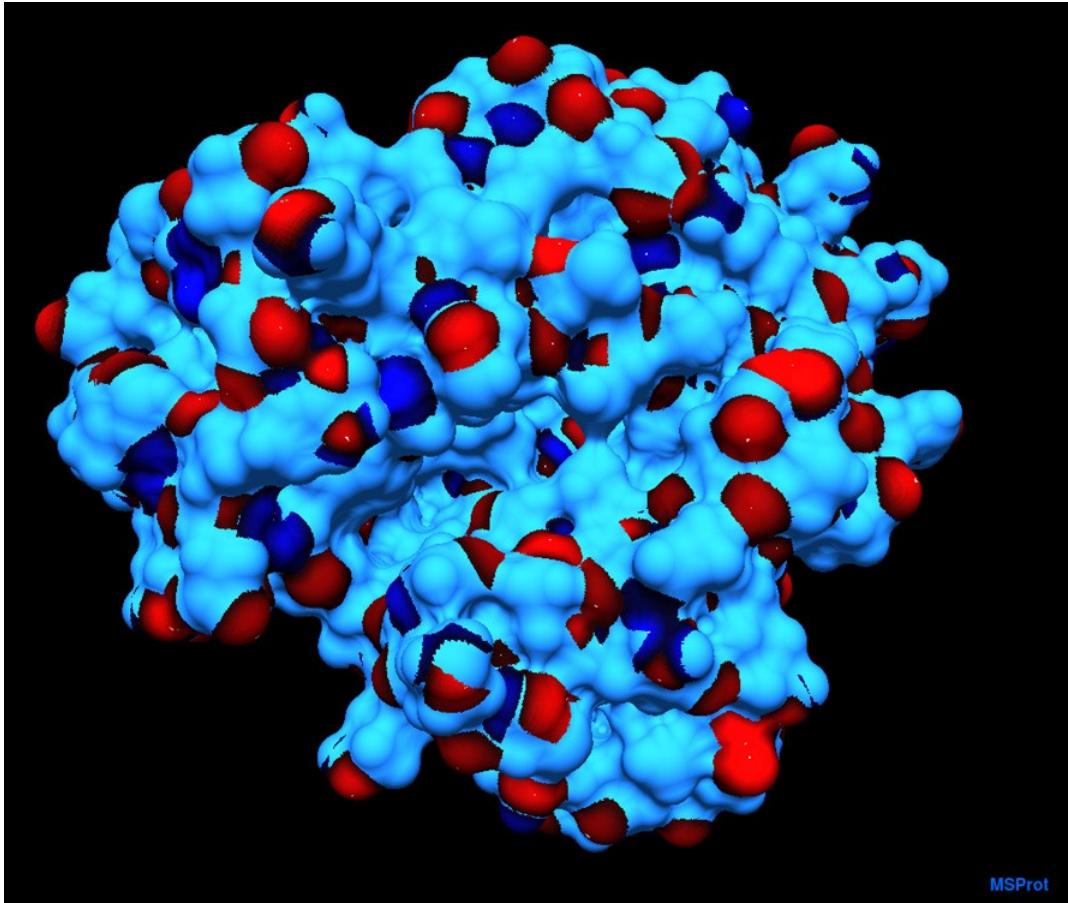


ÁCIDO ASPÁRTICO - ASP



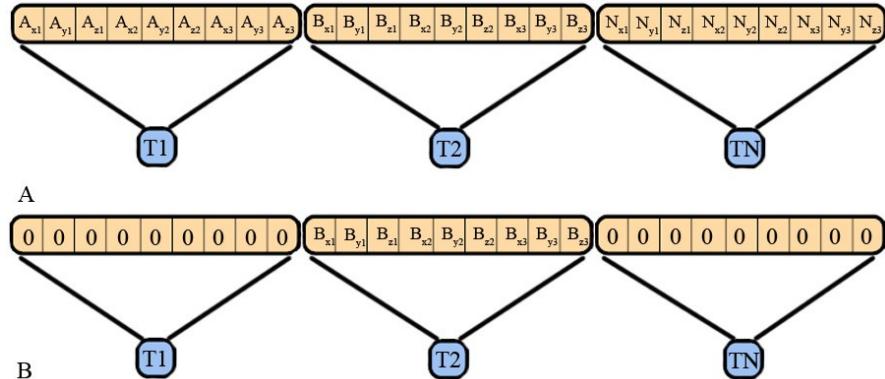
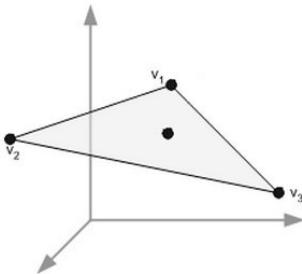
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REGIÕES DOADORAS E ACEPTORAS NA PROTEÍNA



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CÁLCULOS EM CUDA

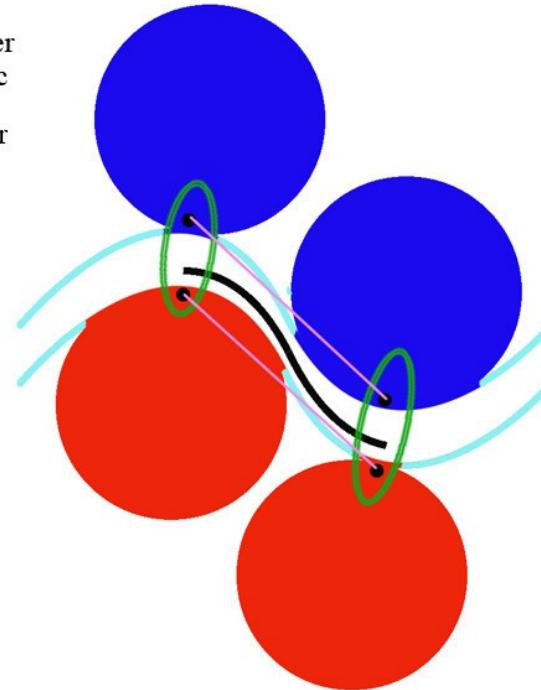


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PROPRIEDADES FÍSICO-QUÍMICAS

- RMSD
- Perimeter
- Geodesic
- Donor
- Acceptor



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3.

Resultados

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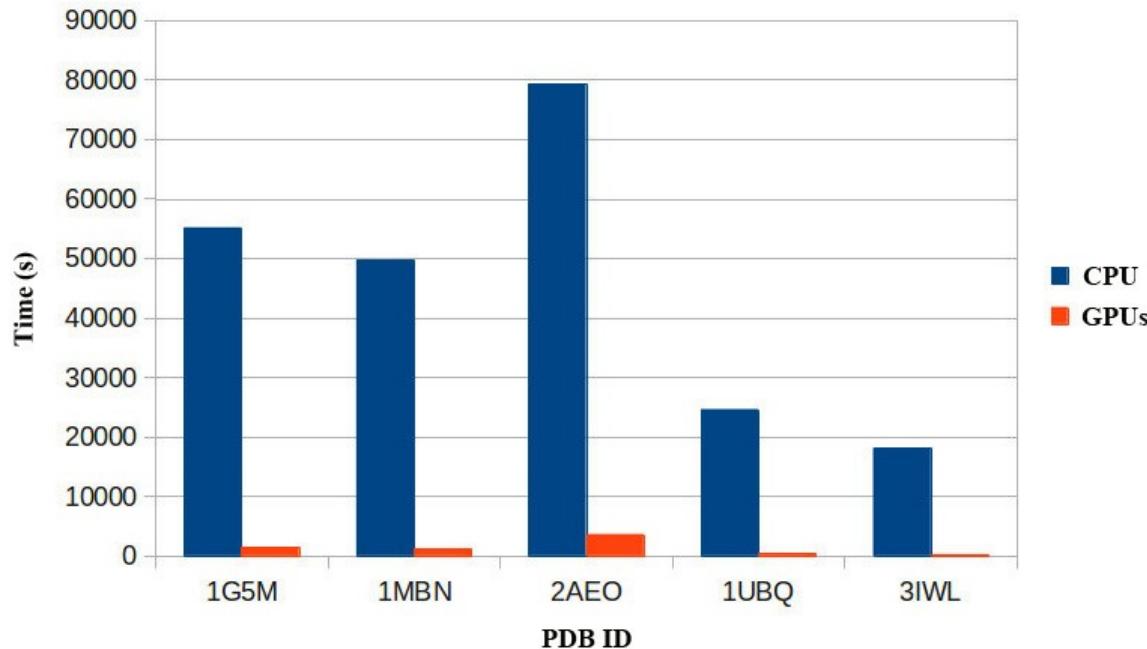


TEMPO DO MAPEAMENTO DAS SUPERFÍCIES

| PDB ID | Number of triangles | Time (s) |
|-------------|---------------------|----------------|
| 1G5M | 10,466,944 | 1457.64 |
| 1MBN | 9,422,144 | 1130.57 |
| 2AEO | 15,059,136 | 3598.5 |
| 1UBQ | 4,667,712 | 353.12 |
| 3IWL | 3,426,496 | 227.54 |

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TEMPO DO MAPEAMENTO DAS SUPERFÍCIES EM CPU E GPUS



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RANKS E LOCAIS FUNCIONAIS DA CISPLATINA

| PDB ID | Rank |
|-------------|----------|
| 1G5M | 2 |
| 1MBN | 1 |
| 2AEO | 3 |
| 1UBQ | 2 |
| 3IWL | 1 |

Qt

| PDB ID | Binding sites | Acceptor atoms | Donated atoms |
|-------------|---------------|----------------|---------------|
| 2AEO | Thr 30 | OG1 | H6 |
| | His 19 | NE2 | H3 |
| 3IWL | Lys 60 | NZ | H3 |
| | Cys 15 | SG | H4 |



THANKS!

The Qt logo, which consists of the letters "Qt" in a white sans-serif font inside a rounded green square.

Any questions?

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