



Acelerando a Descoberta de Novos Fármacos com Qt

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Qt



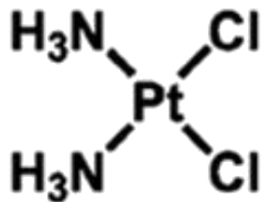
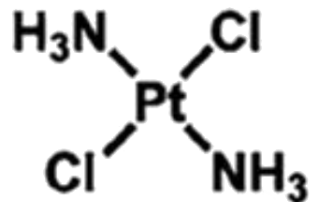
1.

Introdução

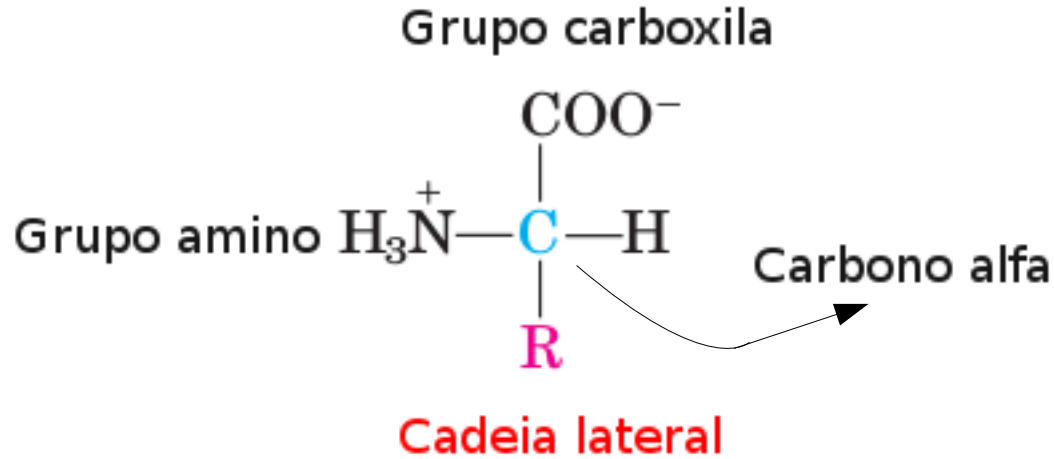
COMPOSTOS BASEADOS EM PLATINA

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.

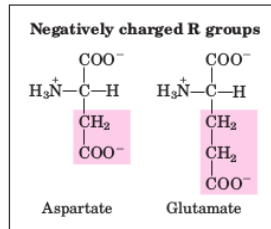
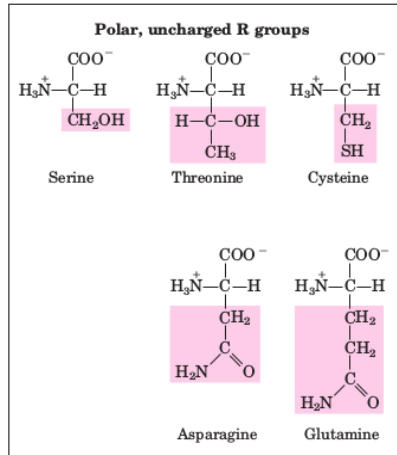
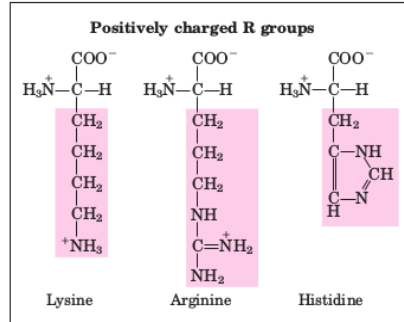
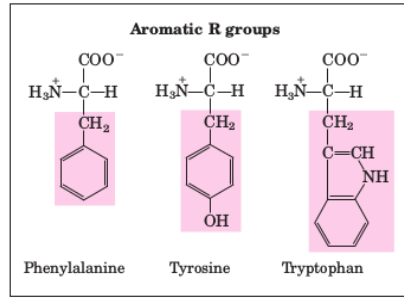
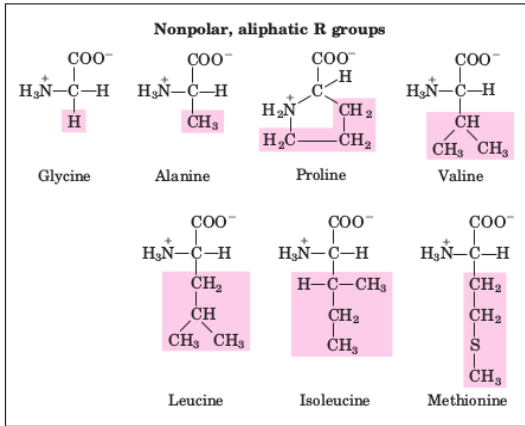
COMPOSTOS BASEADOS EM PLATINA

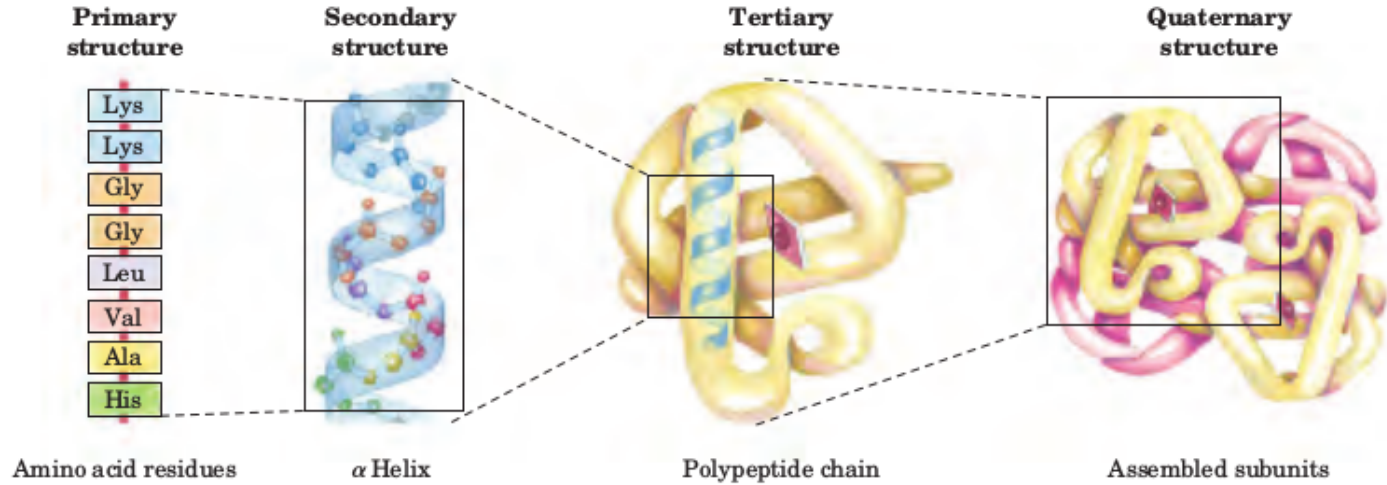
**Cisplatina****Transplatina**

AMINOÁCIDO

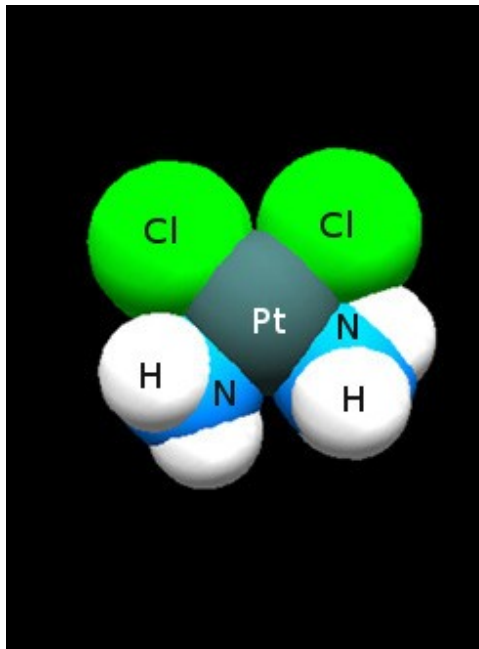


20 TIPOS DE AMINOÁCIDOS

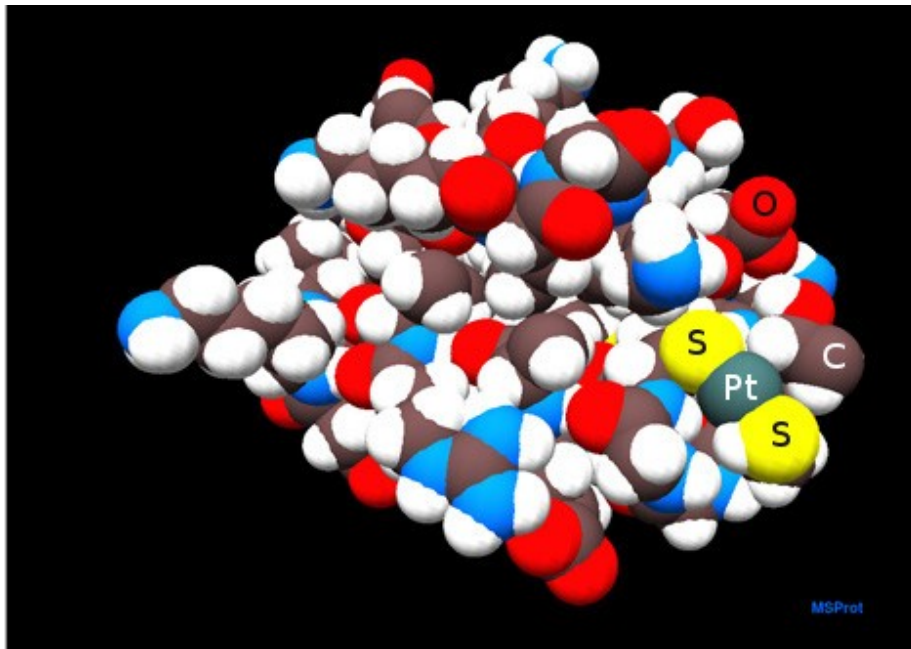


ESTRUTURAS DAS **PROTEÍNAS**

CISPLATINA



CISPLATINA ACOPLADA A PROTEÍNA



Qt

Imagens geradas pelo software **MSProt**.

CISPLATINA ACOPLADA A PROTEÍNA

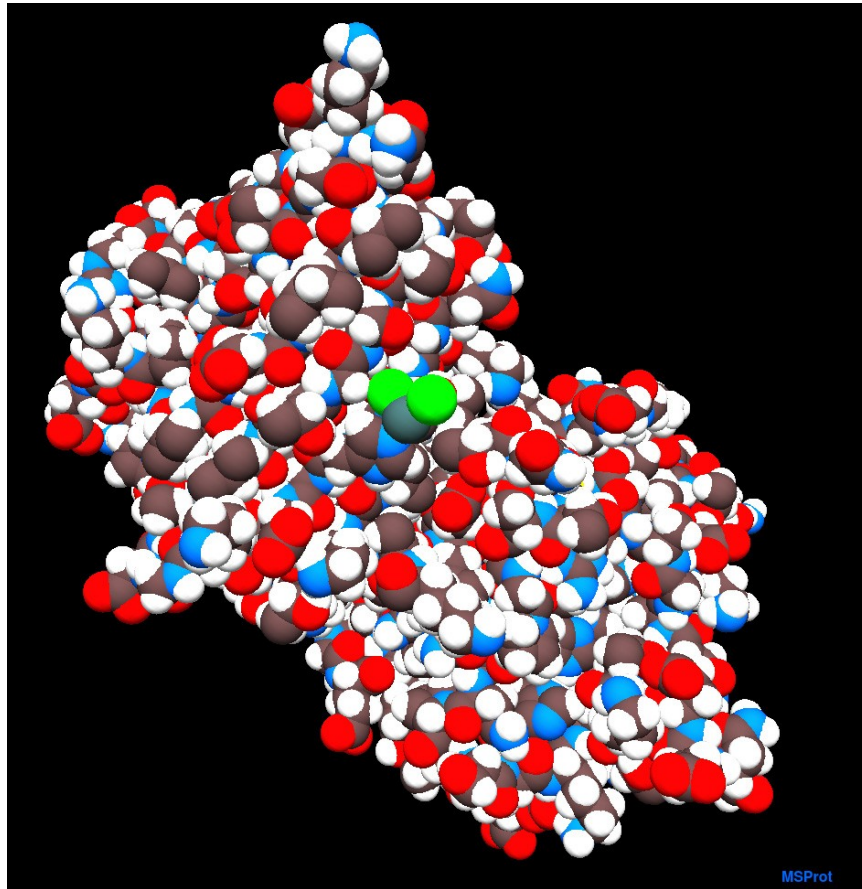


Imagem geradas pelo software **MSProt**.

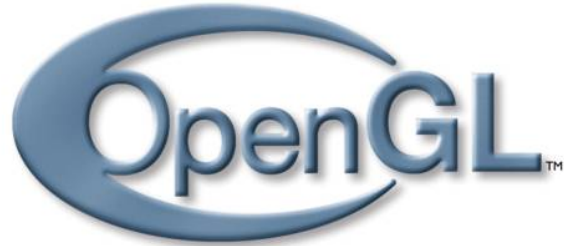
Qt

2.

Materiais e Métodos

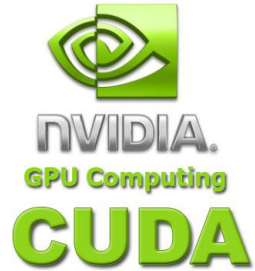


PLATAFORMA DE DESENVOLVIMENTO

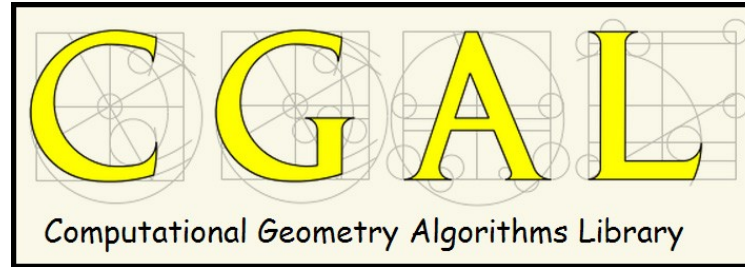


Versão 5.3.1 (LINUX)

PLATAFORMA DE DESENVOLVIMENTO



Versão 5.0



Versão 4.4



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



FUNÇÕES VIRTUAIS

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.



```
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();
        ...
    }
};
```



MSProt em ação!!!

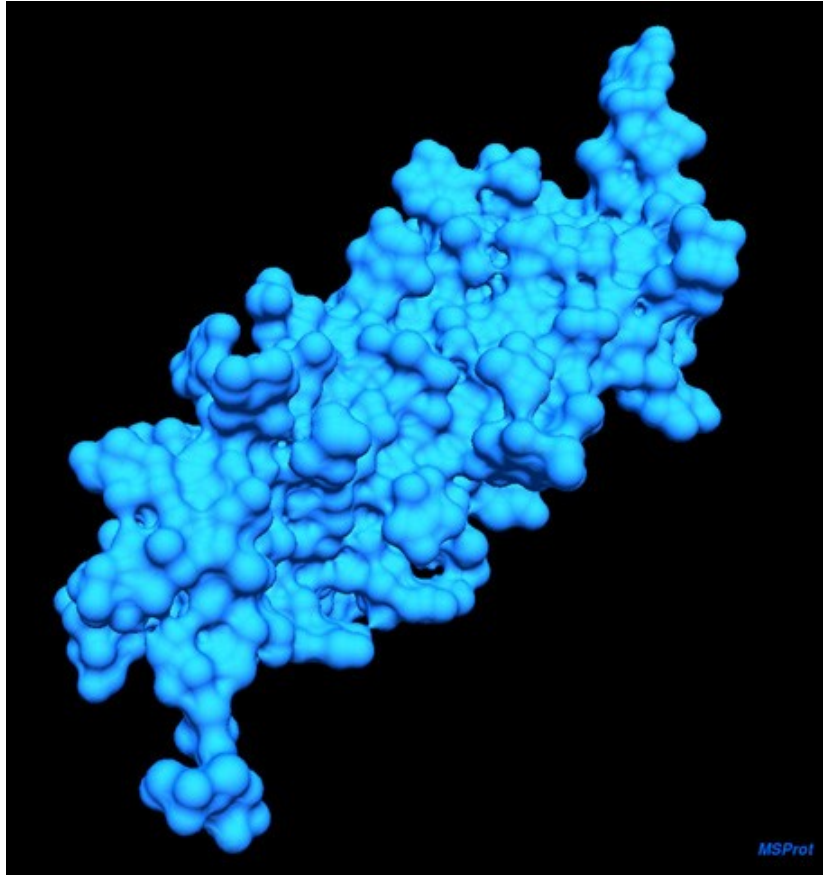
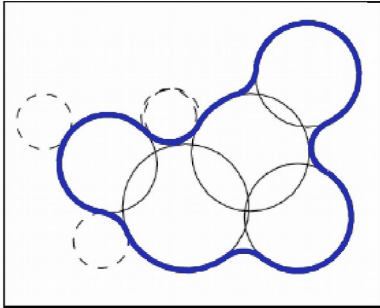
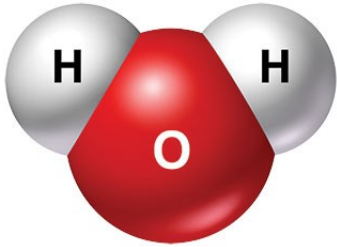
The screenshot displays the MSProt software interface. At the top, a menu bar includes: File, View, Hide atom, Protein, Spheres, Options, Tools, Colors, Surface, Help. The main window shows a 3D ball-and-stick model of a protein structure. Below the model is a table with the following data:

Types	Atom	Amino acid	Chains	N-Amino acid	X	Y	Z	TempFactor	
1	ATOM	N	ASP	A	1	0.970001	-0.579	1.3765	0
2	ATOM	CA	ASP	A	1	0.850001	0.195	0.1395	0
3	ATOM	C	ASP	A	1	1.17	1.671	0.3685	0
4	ATOM	O	ASP	A	1	2.07	2.22	-0.2735	0
5	ATOM	CB	ASP	A	1	-0.549999	0.0549994	-0.4615	0
6	ATOM	CG	ASP	A	1	-1.02	-1.385	-0.4925	0
7	ATOM	OD1	ASP	A	1	-0.349999	-2.22	-1.1325	0
8	ATOM	OD2	ASP	A	1	-2.07	-1.678	0.1205	0
9	ATOM	H	ASP	A	1	1.7	-1.218	1.4735	0
10	ATOM	HA	ASP	A	1	1.57	-0.203001	-0.5605	0
11	ATOM	HB2	ASP	A	1	-1.24	0.631999	0.1255	0
12	ATOM	HB3	ASP	A	1	-0.529999	0.433	-1.4735	0

Below the table, there are several control panels:

- Skin Surface**: Includes a dropdown menu for "Type Surface" (set to "Surface"), a "Skinfactor" input field (0.50), and a "Trianglefactor" input field (2).
- Init**: A range selector from 1 to 12.
- End**: A range selector from 12 to 12.
- Cuda**: A checked checkbox.
- inhibitors**: A dropdown menu set to "None".
- Cargas**: An unchecked checkbox.
- Potencial total**: An unchecked checkbox.
- Build Skin**: A button.
- Max potential**: An unchecked checkbox.
- Mapping**: A button.

SUPERFÍCIE MOLECULAR (SKIN SURFACE)



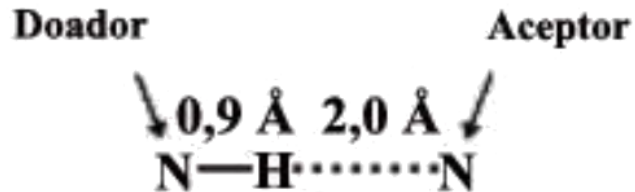
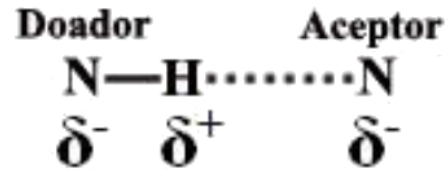
Qt

LIGAÇÕES DE **HIDROGÊNIO**

Aceptor - Aceita um próton de hidrogênio



Doador - Doa um próton de hidrogênio



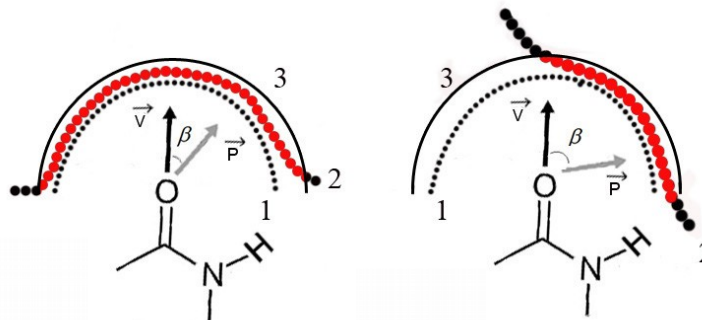
$$1 \text{ \AA} = 10^{-10} \text{ m}$$

MAPEAMENTO DA SUPERFÍCIE MOLECULAR

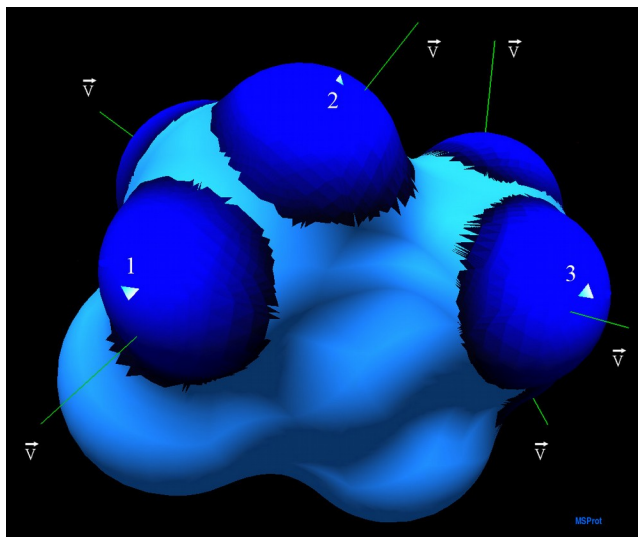
Aceptor - Aceita um próton de hidrogênio



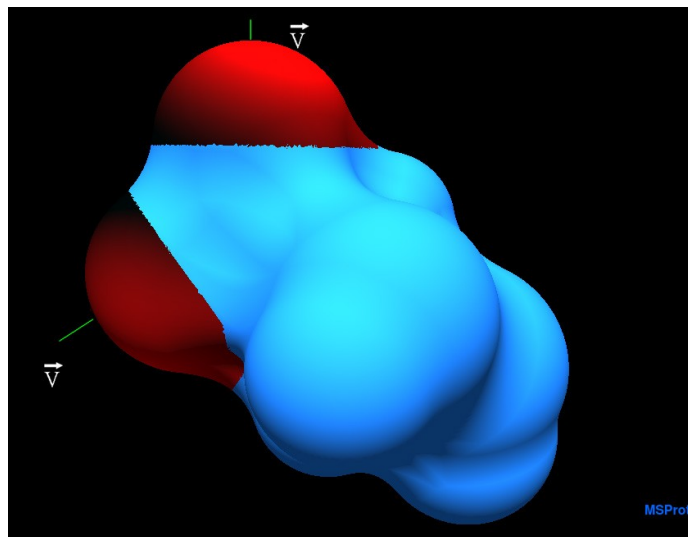
Doador - Doa um próton de hidrogênio



CISPLATINA

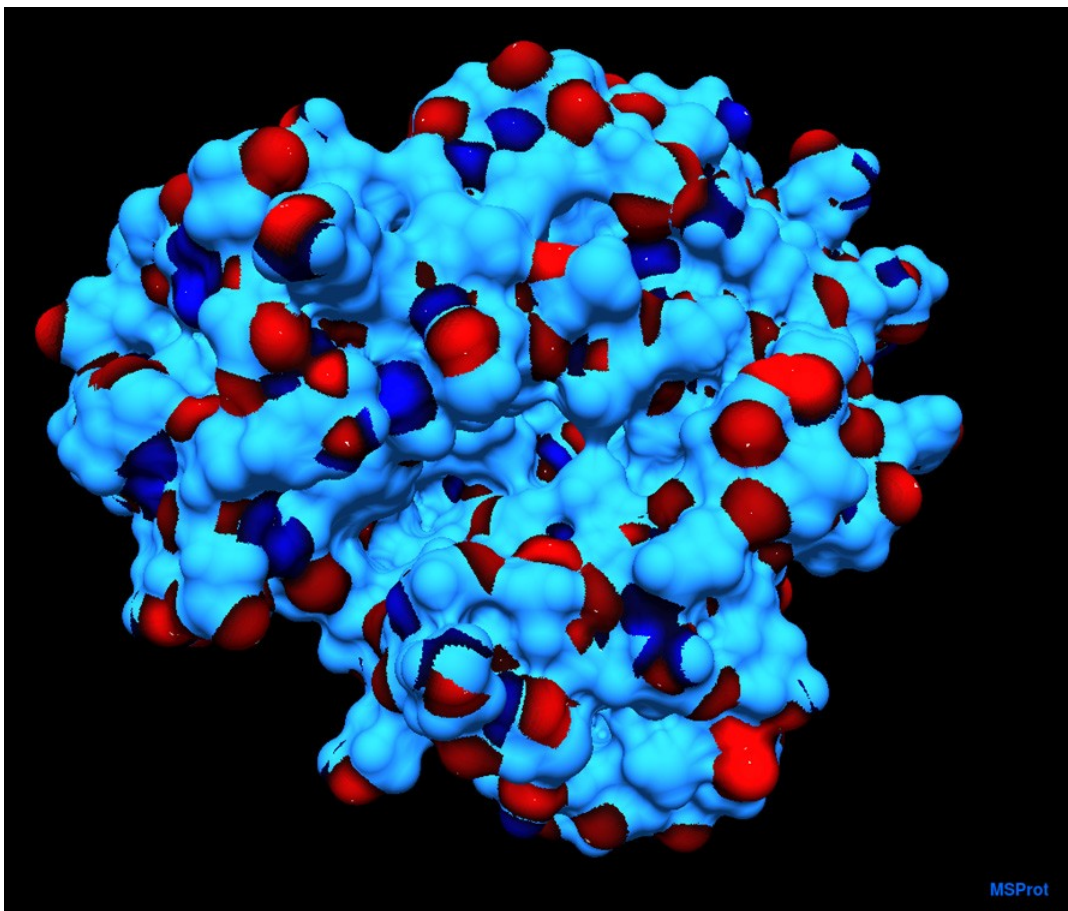


ÁCIDO ASPÁRTICO - ASP



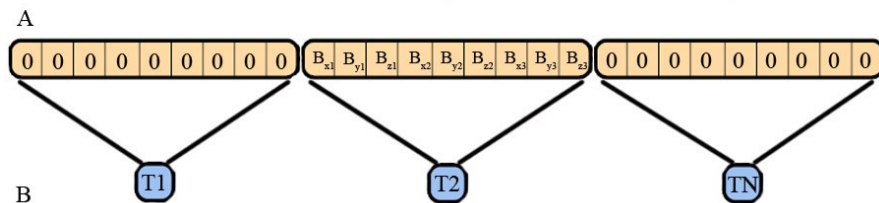
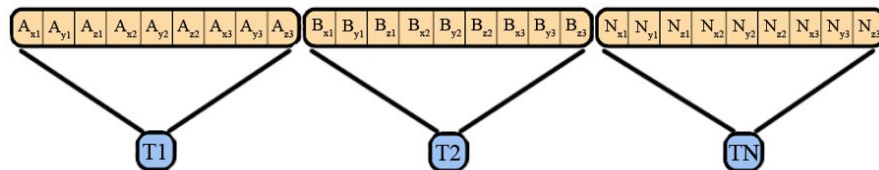
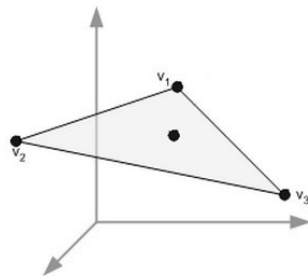
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REGIÕES DOADORAS E ACCEPTORAS NA PROTEÍNA








Qt

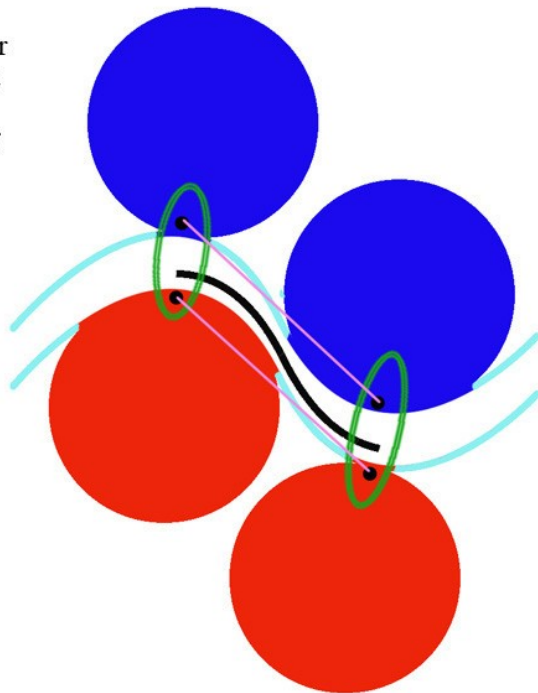
CÁLCULOS EM CUDA





PROPRIEDADES FÍSICO-QUÍMICAS

-  RMSD
-  Perimeter
-  Geodesic
-  Donor
-  Acceptor



Qt

Qt

3.

Resultados

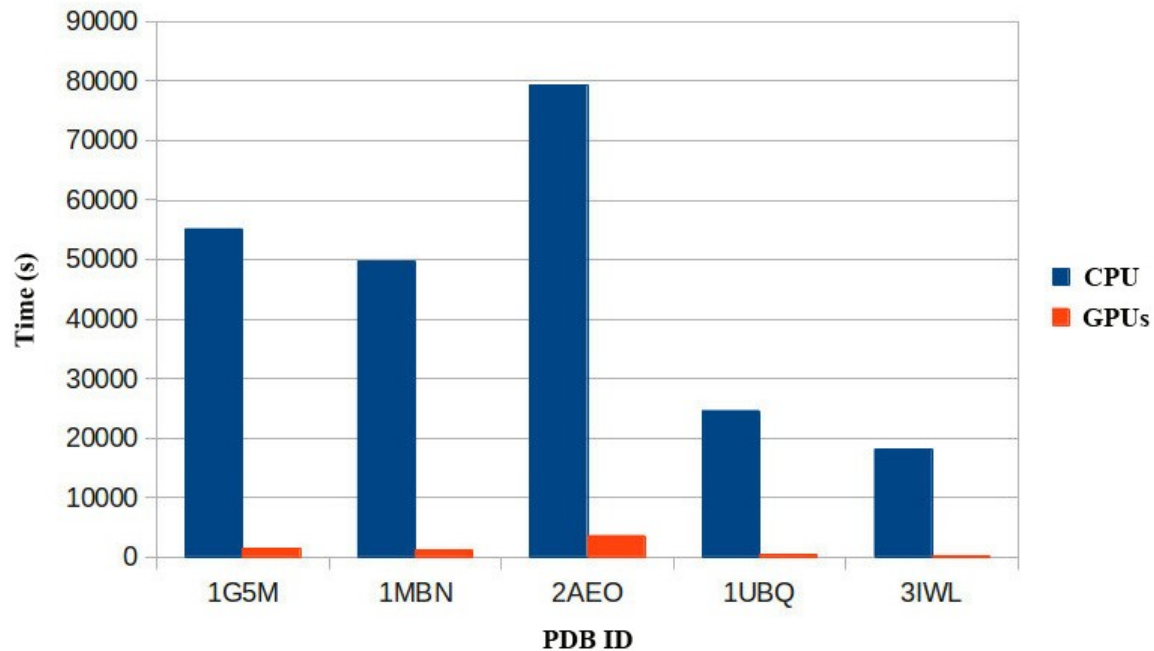




TEMPO DO MAPEAMENTO DAS SUPERFÍCIES

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

TEMPO DO MAPEAMENTO DAS SUPERFÍCIES EM CPU E GPUS





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!

Any questions?

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