Implementazione di algoritmi in linguaggio “Python” per lo sviluppo di modelli 3-D QSAR tramite l’interfacciamento tra UCSF Chimera e il portale www.3d-qsar.com

SAPIENZA
UNIVERSITÀ DI ROMA

Facoltà di Farmacia e Medicina
Corso di laurea magistrale in Biotecnologie Farmaceutiche
Tesi di laurea sperimentale in Chimica Farmaceutica

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Candidato:
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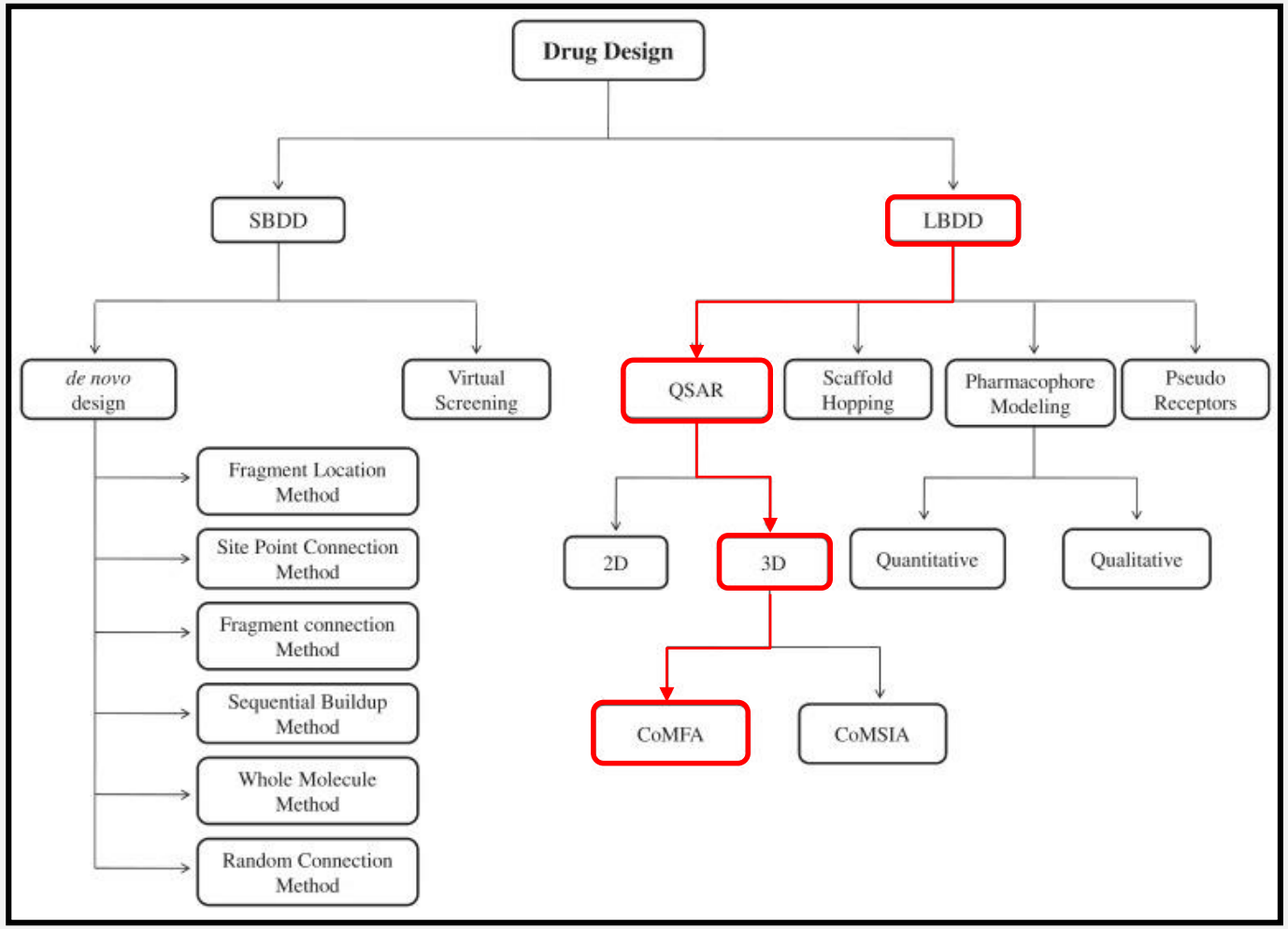
Introduzione

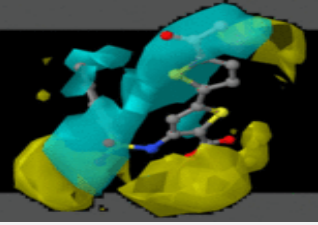


Ligand-**B**ased **D**rug **D**esign

Quantitative **S**tructure-**A**ctivity **R**elationships

3-**D**imensional

Comparative **M**olecular **F**ield **A**nalysis



3-D QSAR

Disegno della struttura 2D della molecola

Marvin Sketch

Trasformazione in struttura 3D

Marvin Sketch / Balloon

Generazione dei conformeri

Balloon

Allineamento dei vari conformeri

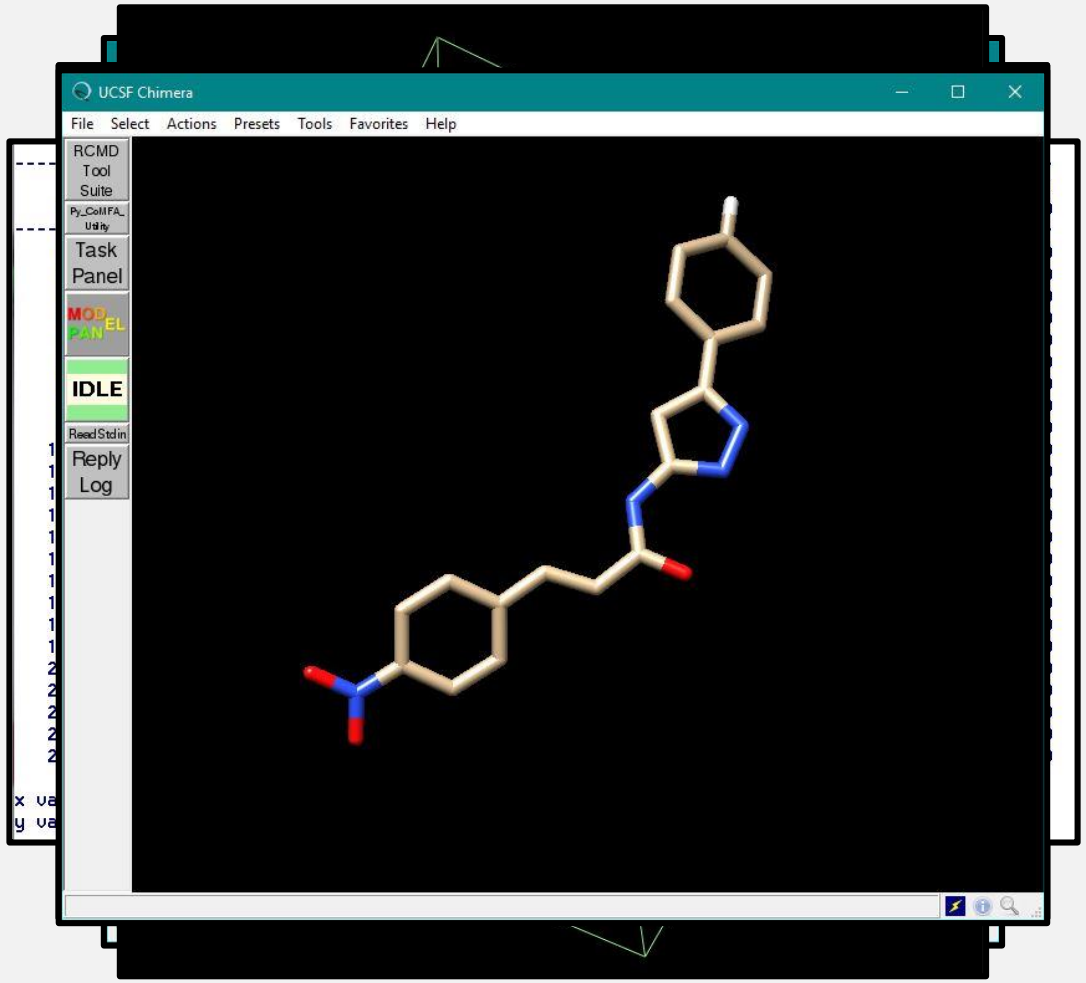
ShaEP

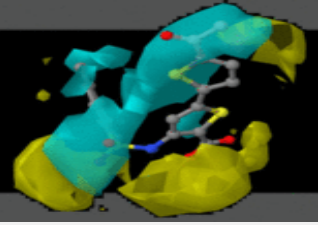
Generazione del modello 3-D QSAR

Py-COMFA

Analisi delle Mappe CoMFA

Chimera

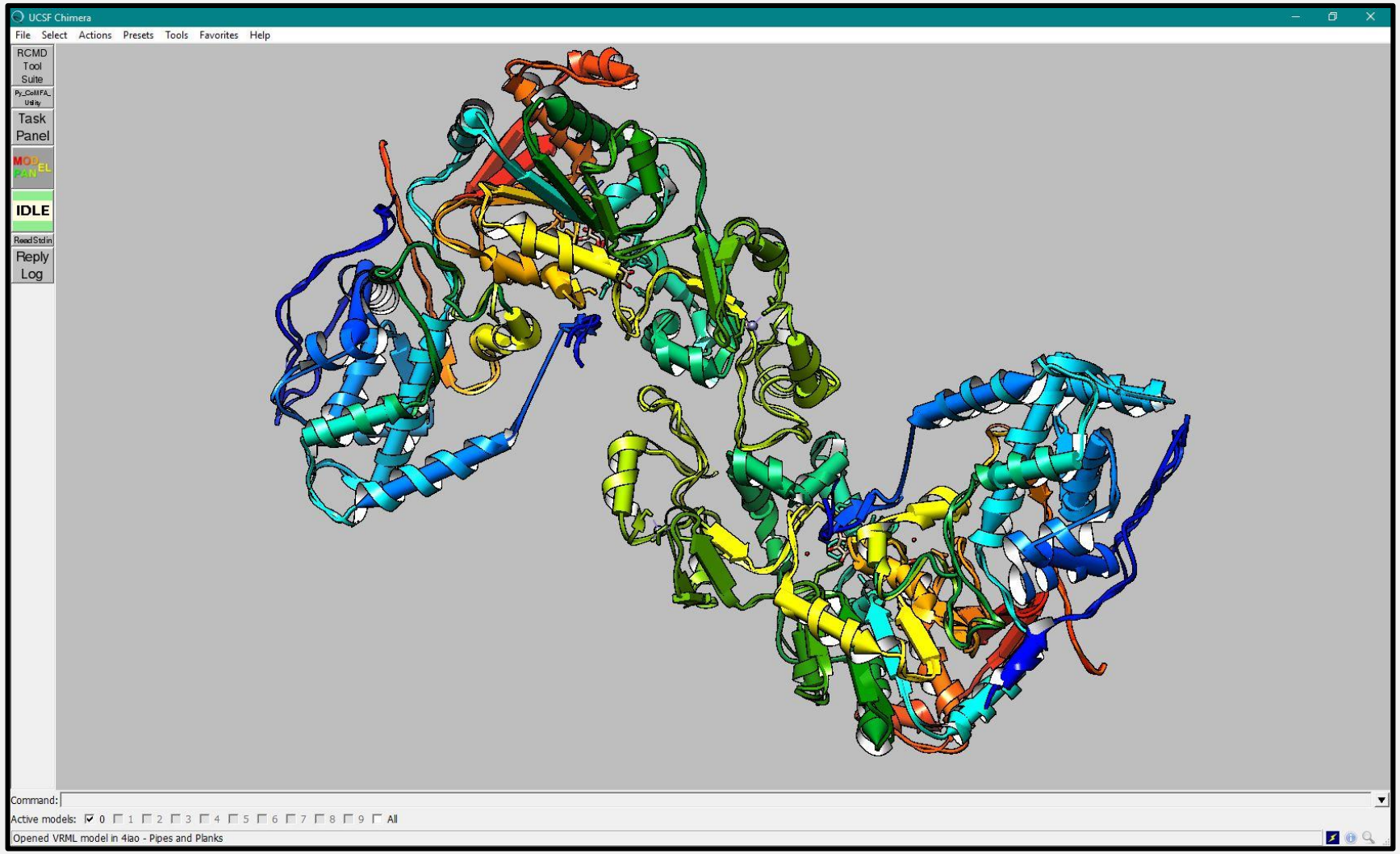


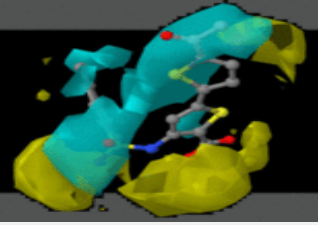


Punti Critici

1. Interfaccia Utente Unificata
2. Prestazioni
3. Esecuzione Remota
4. Facilità Di Utilizzo

UCSF Chimera

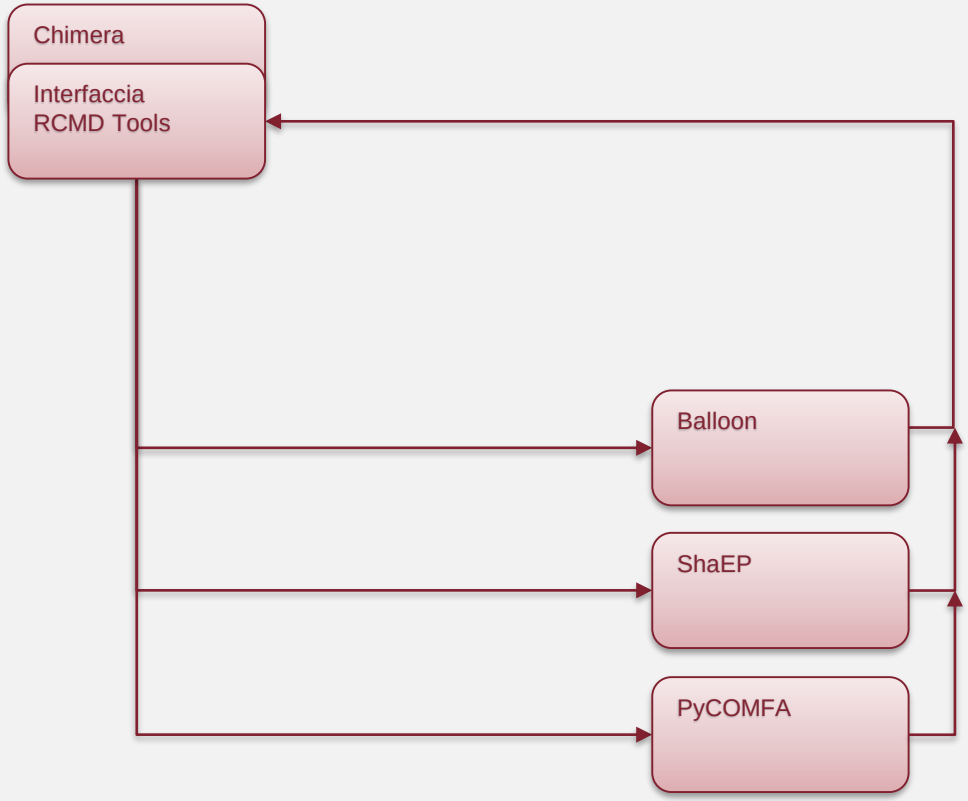




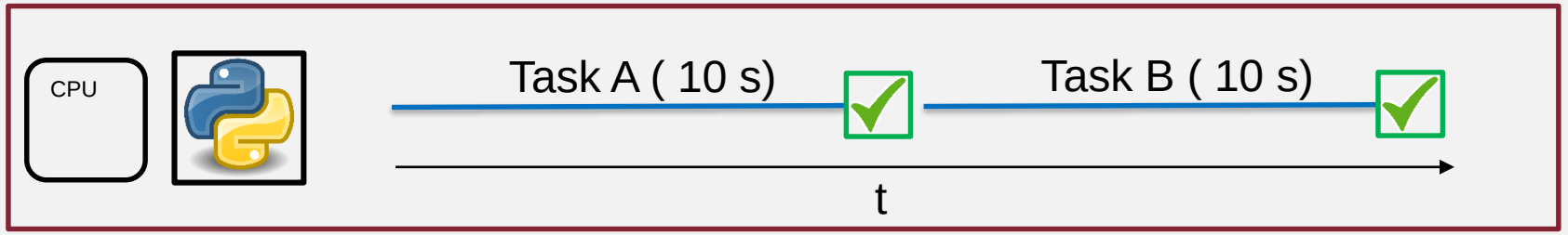
Python

- **Python is:**
- **A high-level programming language**
- **Interpreted**
- **Interactive**
- **Object-Oriented**

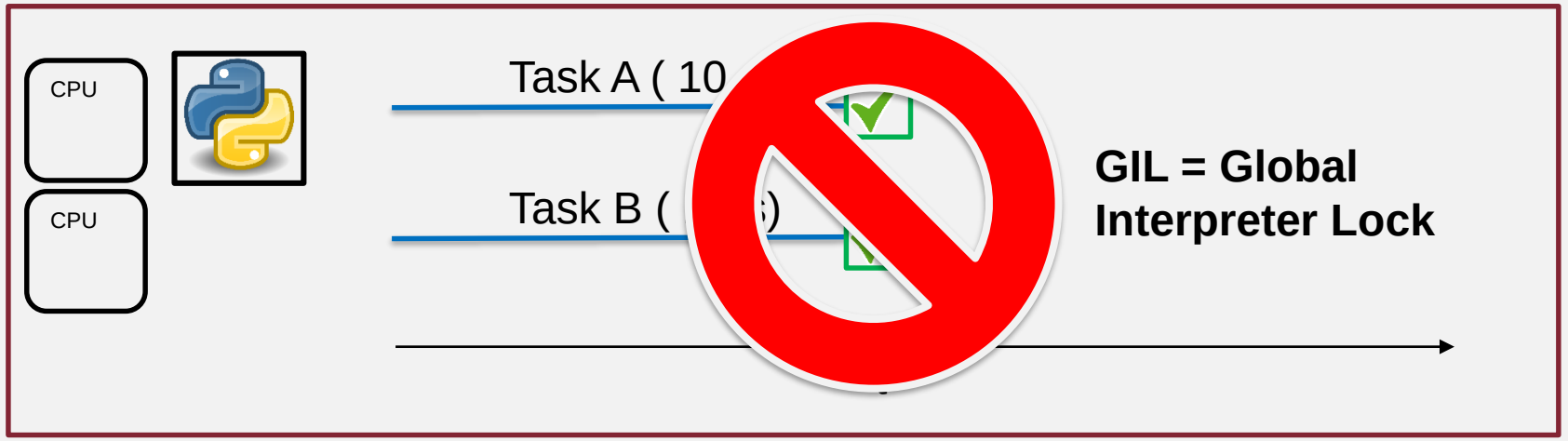
Organizzazione Plug-in



Prestazioni

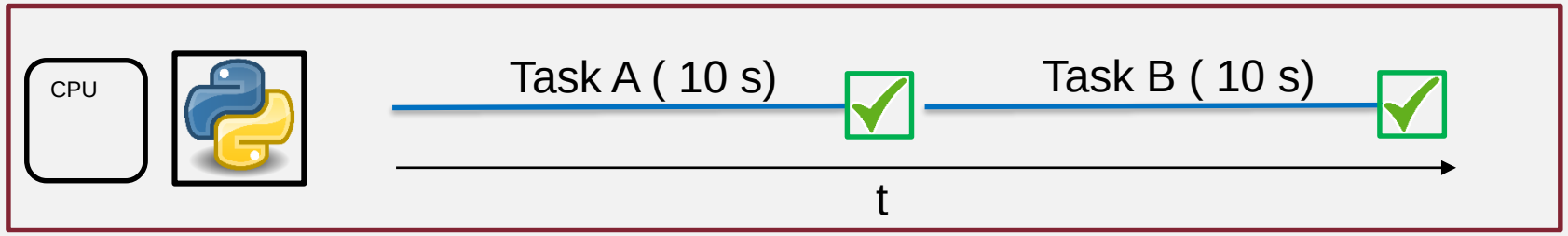


t_{Finale} = A + B = 20 secondi

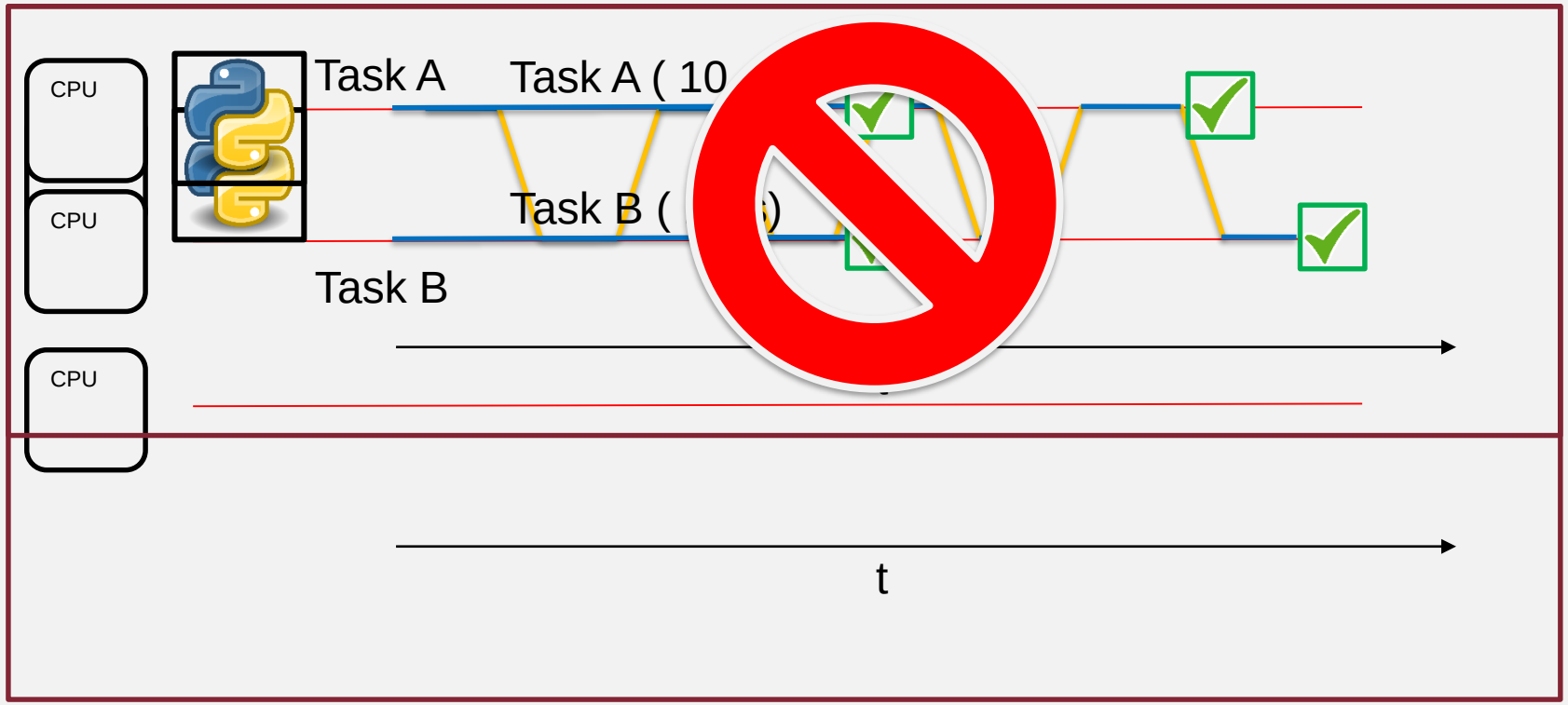


t_{Finale} = A = B = 10 secondi

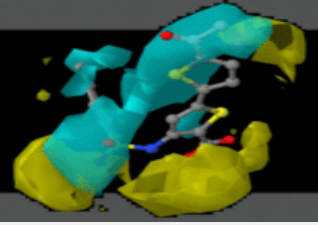
Prestazioni



t_{Finale} = A + B = 20 secondi



t_{Finale} = ?



Prestazioni

```
def count(n):
    while n > 0:
        n -= 1


numero = 90000000


a = datetime.datetime.now().replace(microsecond=0)


count(numero)
count(numero)


b = datetime.datetime.now().replace(microsecond=0)


tempo_finale= b - a
print(«Done in: » + str(tempo_finale))
```

Funzione: Conta da valore X a 0

X = 90 000 000

Tempo Finale = 7 secondi

(3.5 secondi a ciclo)

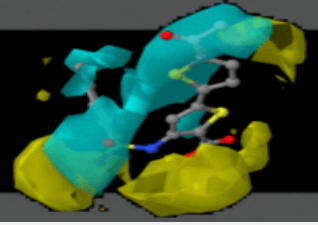
hiamalo A

equenzialmente

Prendi il tempo in secondi, chiamalo B

Tempo finale = B - A

Stampa tempo finale



Prestazioni

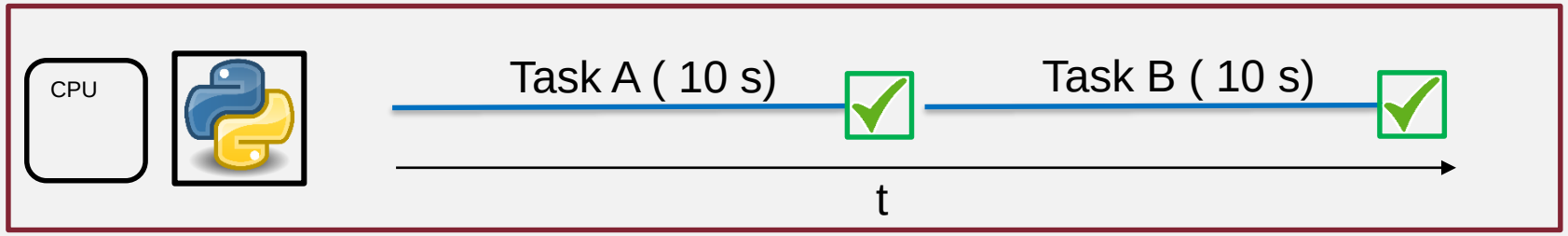
```
def count(n):
    while n > 0:
        n -= 1

numero = 90000000

a = datetime.datetime.now().replace(microsecond=0)

t1 = threading.Thread(target=count, args=(numero,))
t1.start()
t2 = threading.Thread(target=count, args=(numero,))
t2.start()
t1.join(); t2.join()

b = datetime.datetime.now().replace(microsecond=0)

tempo_finale= b - a
print("Finito in:" + str(tempo_finale))
```

Tempo Finale = 14 secondi

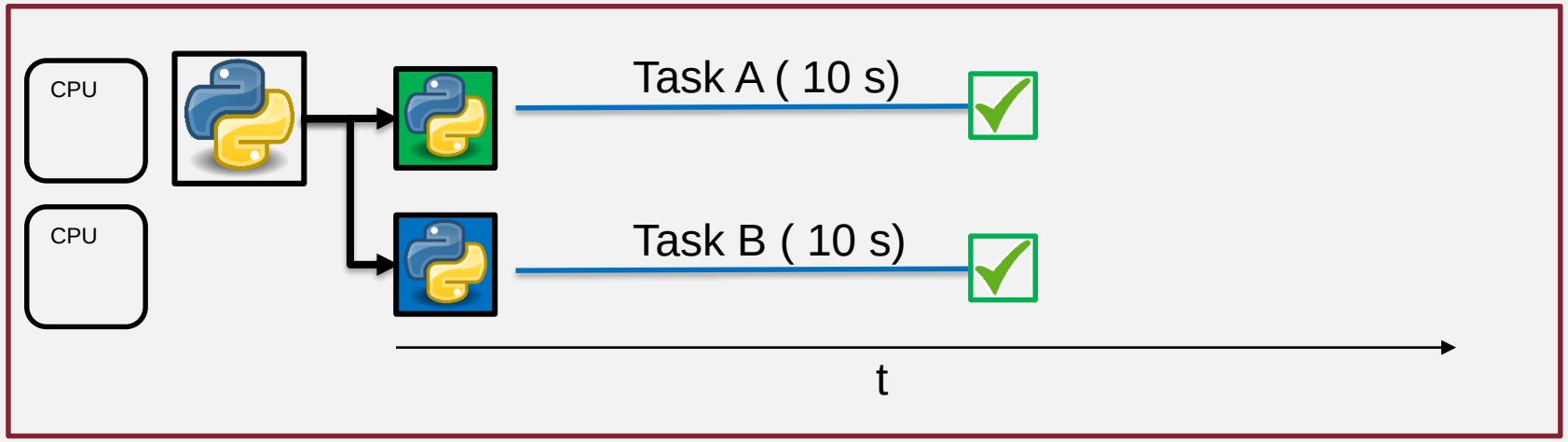
Overhead di 7 secondi!

eseguono 1

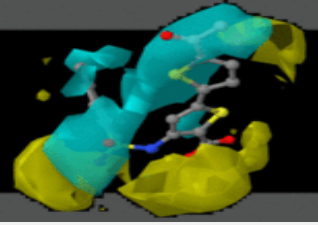
Prestazioni



$t_{Finale} = A + B = 20$ secondi



$t_{Finale} = A = B = 10$ secondi



Prestazioni

```
def count(n):
    while n > 0:
        n -= 1
    print "done"


if __name__ == '__main__':
    numero = 90000000
    a = datetime.datetime.now().replace(microsecond=0)

    p = multiprocessing.Process(target=count, args=(numero,))
    n = multiprocessing.Process(target=count, args=(numero,))

    p.start();n.start()

    p.join(); n.join()

    b = datetime.datetime.now().replace(microsecond=0)
    tempo_finale = b - a

    print("Finito in:" + str(tempo_finale))
```

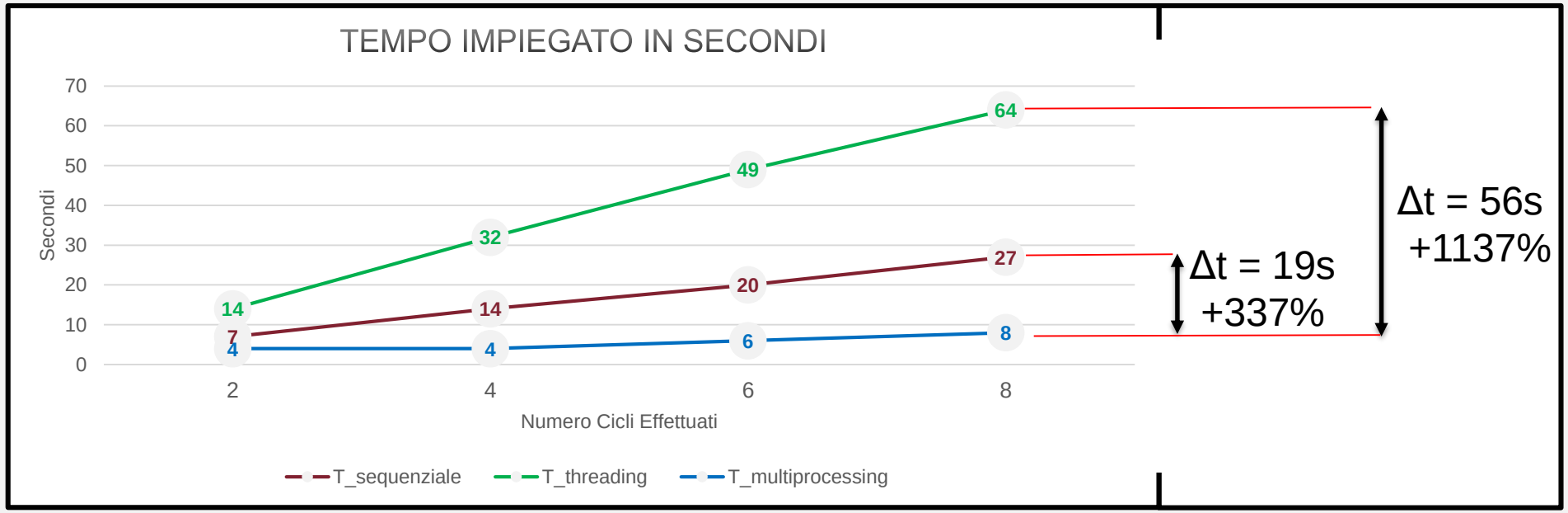
Tempo Finale = 4 secondi

Crea 2 **processi** differenti che eseguono 1 ciclo della funzione ciascuno

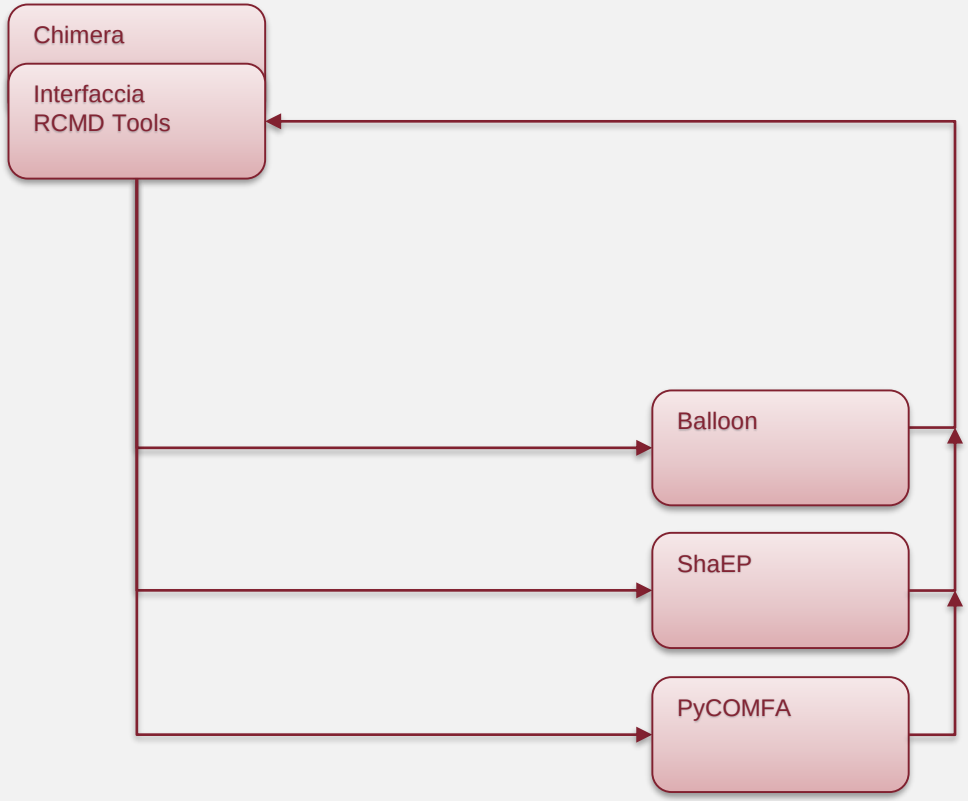
Prestazioni – Dati Conclusivi

CPU a 4 Core

Numero di Cicli	T_sequenziale	T_threading	T_multiprocessing
2	7 secondi	14 secondi	4 secondi
4	14 secondi	32 secondi	4 secondi
6	20 secondi	49 secondi	6 secondi
8	27 secondi	64 secondi	8 secondi



Organizzazione Plug-in



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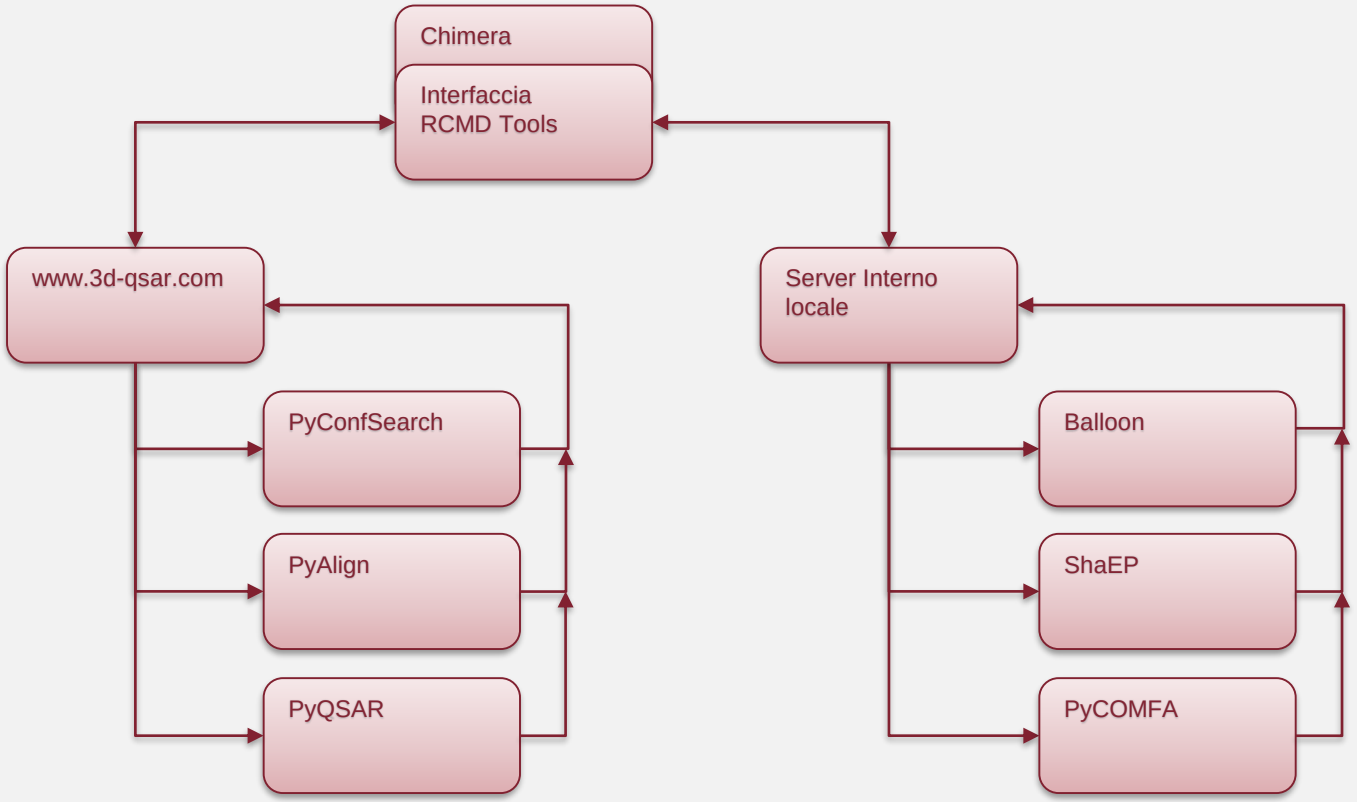
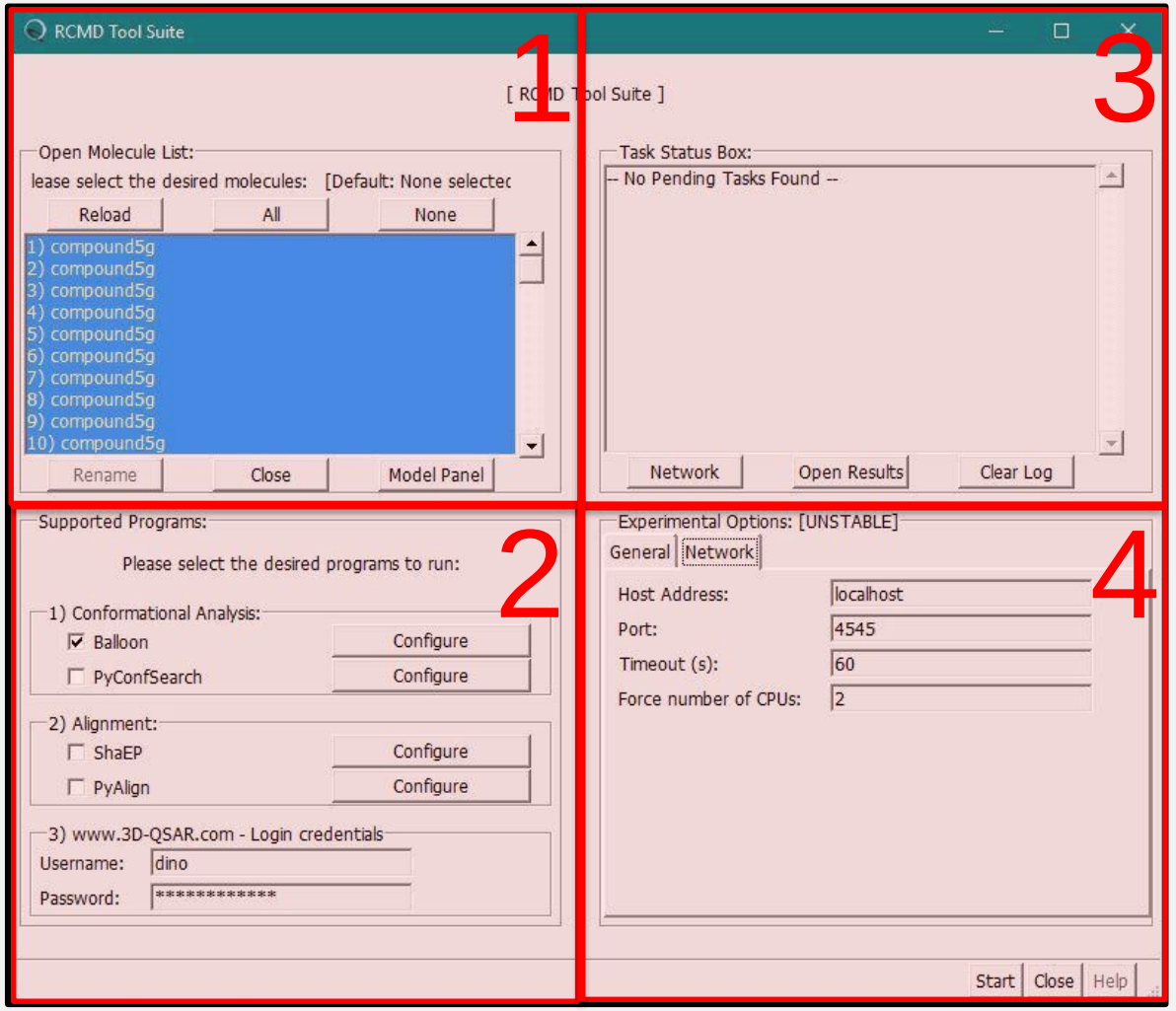
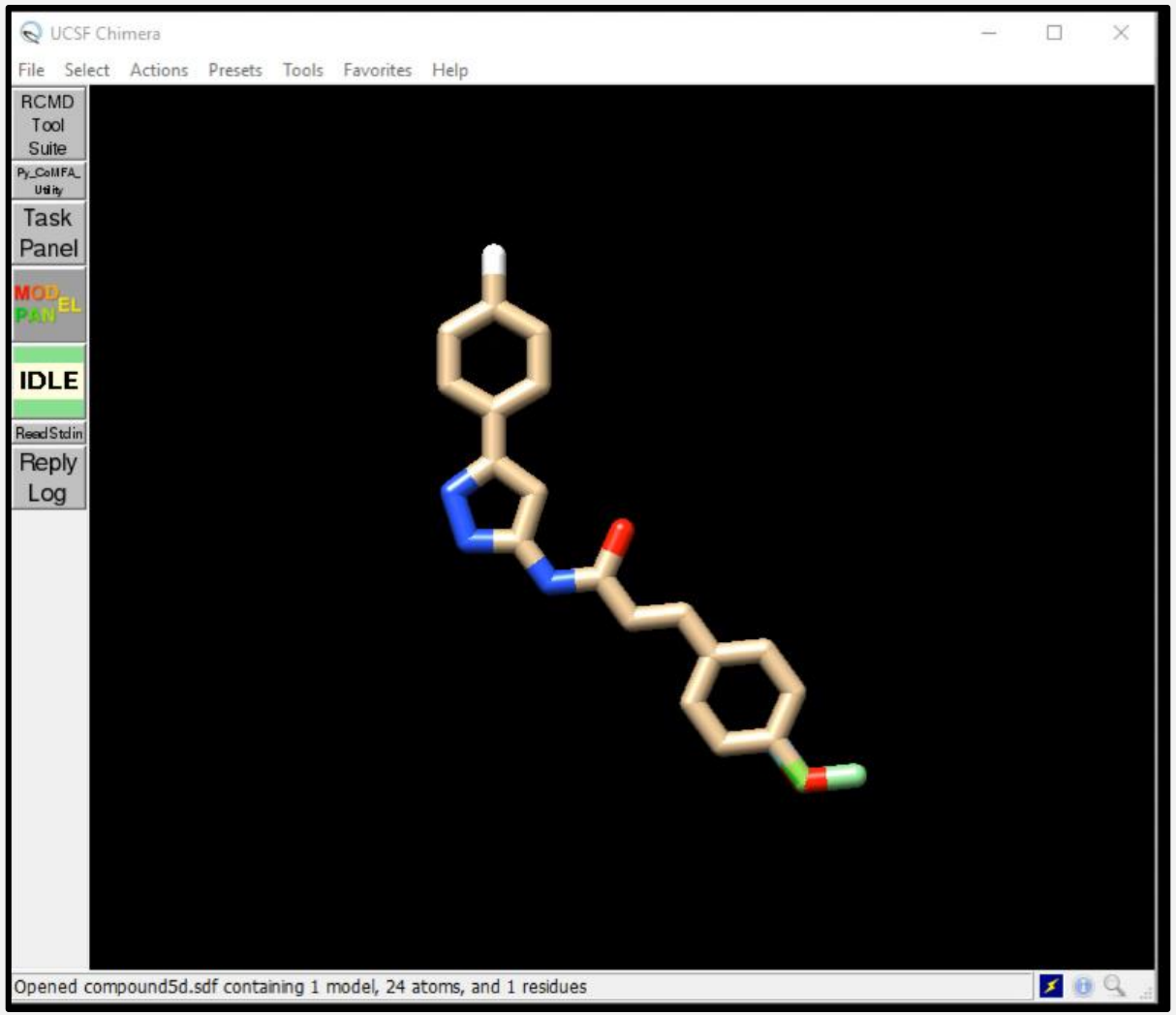
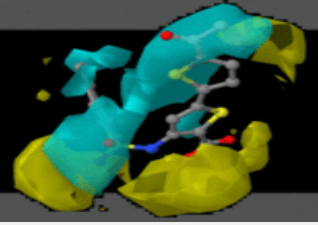


Interfaccia Principale



Esempio di utilizzo





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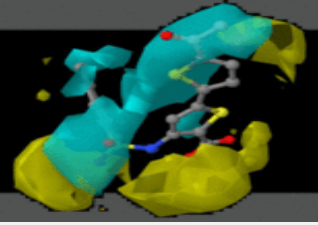

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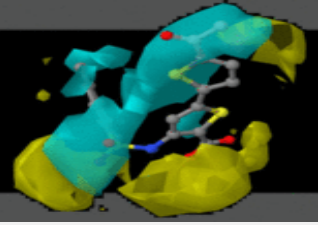

Conclusioni

- Risoluzione dei 4 punti critici presi in considerazione
- Possibilità di espansione a Chromebook e Cellulari
- Altamente modulare e di facile mantenimento
- Nuovo strumento didattico