

Trabalho III

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6 de julho de 2017

Sumário

- 1 Prelúdio
- 2 Criação da proteína
- 3 Implementação
- 4 Resultados

Antes de começar...

Correção da formatação do arquivo PDB do trabalho II.

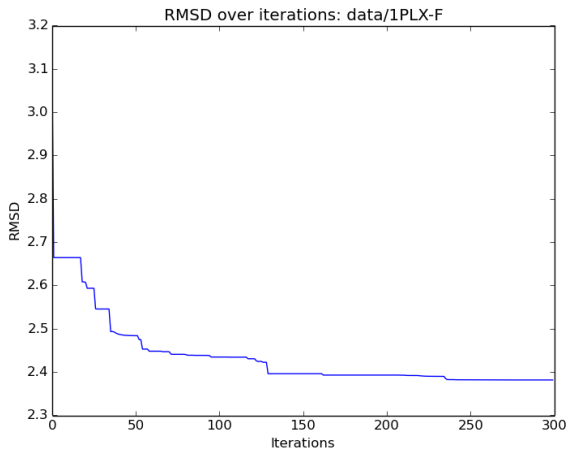
1	ATOM	1	N	TYR	1	0.808	0.808	0.000	1.00	0.00
2	ATOM	2	CA	TYR	1	1.459	0.858	0.000	1.00	0.00
3	ATOM	3	C	TYR	1	1.944	1.488	0.000	1.00	0.00
4	ATOM	4	O	TYR	1	1.164	2.442	0.000	1.00	0.00
5	ATOM	5	CB	TYR	1	2.042	-0.648	-1.259	1.00	0.00
6	ATOM	6	CG	TYR	1	1.741	-2.143	-1.412	1.00	0.00
7	ATOM	7	CD1	TYR	1	2.452	-3.693	-0.673	1.00	0.00
8	ATOM	8	CD2	TYR	1	0.739	-2.563	-2.292	1.00	0.00
9	ATOM	9	CE1	TYR	1	2.158	-4.448	-0.810	1.00	0.00
10	ATOM	10	CE2	TYR	1	0.447	-3.917	-2.428	1.00	0.00
11	ATOM	11	CZ	TYR	1	1.157	-0.858	-1.686	1.00	0.00
12	ATOM	12	OH	TYR	1	0.870	-6.188	-1.815	1.00	0.00
13	ATOM	13	1H	TYR	1	-0.608	0.893	0.000	1.00	0.00
14	ATOM	14	2H	TYR	1	-0.536	-0.937	0.000	1.00	0.00
15	ATOM	15	HA	TYR	1	1.037	-0.429	0.918	1.00	0.00
16	ATOM	16	1HB	TYR	1	1.769	-0.108	-2.170	1.00	0.00
17	ATOM	17	2HB	TYR	1	3.143	-0.527	-1.277	1.00	0.00
18	ATOM	18	HD1	TYR	1	3.227	-2.783	0.014	1.00	0.00
19	ATOM	19	HD2	TYR	1	0.175	-1.637	-2.063	1.00	0.00
20	ATOM	20	HE1	TYR	1	2.701	-5.182	-0.234	1.00	0.00
21	ATOM	21	HE2	TYR	1	-0.334	-4.227	-3.106	1.00	0.00
22	ATOM	22	HH	TYR	1	0.161	-6.284	-2.453	1.00	0.00
23	ATOM	23	N	GLY	2	3.254	1.654	0.000	1.00	0.00
24	ATOM	24	CA	GLY	2	3.819	3.000	-0.000	1.00	0.00
25	ATOM	25	C	GLY	2	5.328	2.954	-0.000	1.00	0.00
26	ATOM	26	O	GLY	2	5.946	1.894	0.000	1.00	0.00
27	ATOM	27	1H	GLY	2	3.672	2.656	-0.000	1.00	0.00
28	ATOM	28	1HA	GLY	2	3.473	3.561	-0.888	1.00	0.00
29	ATOM	29	2HA	GLY	2	3.473	3.561	0.888	1.00	0.00
30	ATOM	30	N	GLY	3	5.943	4.122	-0.000	1.00	0.00
31	ATOM	31	CA	GLY	3	7.402	4.178	-0.000	1.00	0.00
32	ATOM	32	C	GLY	3	7.889	5.608	-0.000	1.00	0.00
33	ATOM	33	O	GLY	3	7.113	6.558	-0.000	1.00	0.00
34	ATOM	34	1H	GLY	3	7.023	4.164	-0.000	1.00	0.00
35	ATOM	35	1HA	GLY	3	7.805	3.657	0.888	1.00	0.00
36	ATOM	36	2HA	GLY	3	7.805	3.657	-0.888	1.00	0.00
37	ATOM	37	N	PHE	4	9.129	5.773	-0.000	1.00	0.00
38	ATOM	38	CA	PHE	4	9.764	7.120	-0.000	1.00	0.00
39	ATOM	39	C	PHE	4	11.274	7.073	-0.000	1.00	0.00
40	ATOM	40	O	PHE	4	11.909	5.982	0.000	1.00	0.00
41	ATOM	41	CG	PHE	4	9.284	7.901	1.261	1.00	0.00
42	ATOM	42	CD	PHE	4	7.760	8.951	1.436	1.00	0.00
43	ATOM	43	CD1	PHE	4	7.046	7.062	2.117	1.00	0.00
44	ATOM	44	CD2	PHE	4	7.883	9.131	0.870	1.00	0.00
45	ATOM	45	CE1	PHE	4	5.602	7.143	2.214	1.00	0.00
46	ATOM	46	CE2	PHE	4	5.698	9.217	0.977	1.00	0.00
47	ATOM	47	CZ	PHE	4	4.987	8.222	1.646	1.00	0.00
48	ATOM	48	1H	PHE	4	9.852	4.913	0.000	1.00	0.00
49	ATOM	49	HA	PHE	4	9.437	7.645	-0.917	1.00	0.00
50	ATOM	50	1HB	PHE	4	9.705	7.428	2.173	1.00	0.00
51	ATOM	51	2HB	PHE	4	9.730	8.911	1.262	1.00	0.00
52	ATOM	52	HD1	PHE	4	7.560	6.205	2.533	1.00	0.00
53	ATOM	53	HD2	PHE	4	7.576	8.895	0.331	1.00	0.00

Otimização

Particle Swarm Optimization

- Minimização
- Função de avaliação: $RMSD_{all}$
- Dimensões: $2 \times \|AA\| - 2$
- Limites: $[-\pi, \pi]$
- População: 200
- Iterações: 300

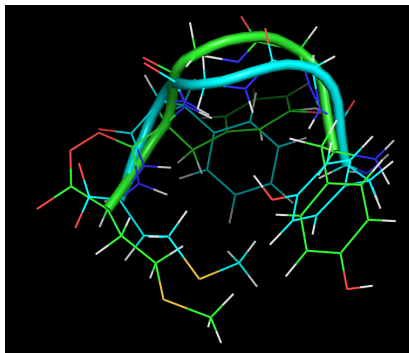
Minimização do RMSD



Tempo de execução: 19 minutos

Resultados

- $RMSD_{C_{\alpha}}$: 0.40Å
- $RMSD_{backbone}$: 0.83Å
- $RMSD_{all}$: 2.38Å



Ângulos (1PLX x 1PLX-F)

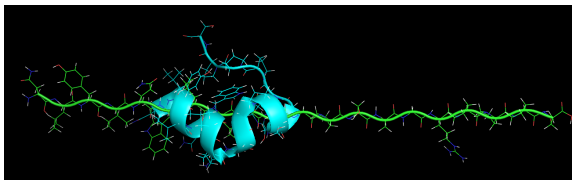
AA	PHI	PSI	OMEGA
TYR	360.00 x 360.00	176.63 x -115.80	360.00 x 360.00
GLY	148.48 x 121.15	-21.96 x 10.17	179.86 x 179.98
GLY	114.02 x 78.37	29.89 x 35.39	179.81 x -179.99
PHE	-88.00 x -81.96	-38.16 x -93.28	179.75 x 179.97
MET	-74.24 x -9.66	360.00 x 360.00	-179.95 x 180.00

Ferramentas

- Python;
- Numpy;
- Orientado a Objetos;
- Trabalhos I e II.

1L2Y

- Sequência: NLYIQWLKDGGPSSGRPPPS;
- 1L2Y x 1L2Y-P:
 - $RMSD_{C_{\alpha}}$: 17.89Å
 - $RMSD_{backbone}$: 18.08Å
 - $RMSD_{all}$: 19.13Å



Energia Potencial (AMBER99)

$$\begin{aligned} E_{total} = & \sum_{bonds} K_b (b - b_0)^2 + \\ & \sum_{UB} K_{UB} (S - S_0)^2 + \\ & \sum_{angle} K_\theta (\theta - \theta_0)^2 + \\ & \sum_{dihedrals} K_\chi (1 + \cos(\eta - \delta)) + \\ & \sum_{impropers} K_{imp} (\varphi - \varphi_0)^2 + \\ & \sum_{nonbond} \varepsilon_{ij} \left[\left(\frac{R_{minij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{minij}}{r_{ij}} \right)^6 \right] + \varepsilon_1 \frac{q_i q_j}{r_{ij}} \end{aligned}$$

Termos não ligados

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

$$R_{mini} = \sigma_i \cdot 2^{1/6}$$

$$r_{ij} = \| P_i - P_j \| / 10 (nm)$$

$$R_{minij} = \frac{R_{mini} + R_{minj}}{2}$$

$$U_{ij}^{LJ} = \sqrt{\varepsilon_i \varepsilon_j} \left[\left(\frac{R_{mini} + R_{minj}}{2r_{ij}} \right)^{12} - 2 \left(\frac{R_{mini} + R_{minj}}{2r_{ij}} \right)^6 \right]$$

$$\varepsilon_1 = 9 \cdot 10^9 \cdot \frac{(1.6022 \cdot 10^{-19})^2}{1 \cdot 10^{-9}} \cdot \frac{6.022140857 \cdot 10^{23}}{1000} (kJ/mol)$$

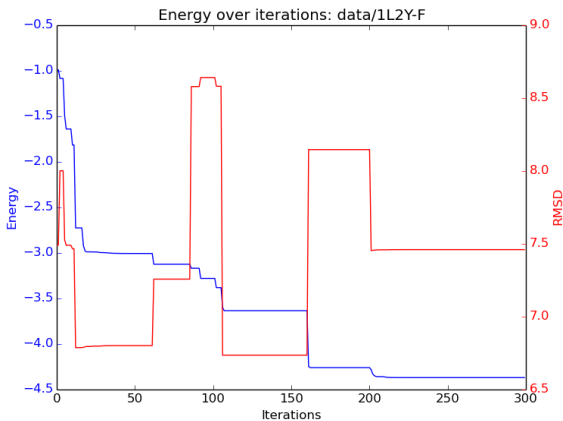
$$E_{nonbond} = \sum_{nonbond} \varepsilon_{ij} \left[\left(\frac{R_{minij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{minij}}{r_{ij}} \right)^6 \right] + \varepsilon_1 \frac{q_i q_j}{r_{ij}}$$

Otimização

Particle Swarm Optimization

- Minimização;
- Função de avaliação: $E_{nonbond}$ (AMBER99);
- Dimensões: $2 \times \|AA\| - 2$;
- Limites: $[-\pi, \pi]$;
- População: 60;
- Iterações: 200

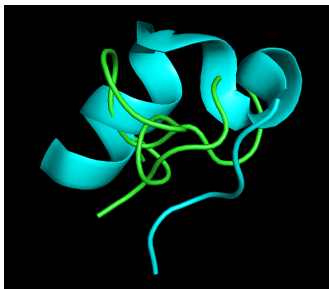
Energia X RMSD



Tempo:

1L2Y X 1L2Y-F

- $E_{nonbond}^{1L2Y} : kJ/mol$
- $E_{nonbond}^{1L2Y-F} : kJ/mol$



- $RMSD_{C_{\alpha}} : \text{\AA}$
- $RMSD_{backbone} : \text{\AA}$
- $RMSD_{all} : \text{\AA}$

Fim