1 Les protocoles

1.1 Les protocoles Monte Carlo

Nom	Temp	Traj (mega)	seuil voisin	Proba
MC0	0.01	6000	0	0 ; 1 ; 0.1 ; 0
MC0-	0.01	300	0	0 ; 1 ; 0.1 ; 0
MC4	0.2	6000	0	0 ; 1 ; 0.1 ; 0
MC4-	0.2	300	0	0 ; 1 ; 0.1 ; 0
MC42	0.2	6000	0	1 ; 0 ; 0.1 ; 0
MC42-	0.2	300	0	1 ; 0 ; 0.1 ; 0

TABLE 1 – Les protocoles Monte Carlo

1.2 Les protocoles Replica Exchange

Nom	marcheurs	Temp	Traj (mega)	seuil voisin	Proba	swap period (mega)
RE1	4	10<->0.01	1500	10	1 ; 0 ; 0.1 ; 0	7.5
RE2	4	1<->0.125	1500	10	1 ; 0 ; 0.1 ; 0	7.5
RE2-	4	1<->0.125	250	10	1 ; 0 ; 0.1 ; 0	2.5
RE22	4	2<->0.25	1500	10	1 ; 0 ; 0.1 ; 0	7.5
RE3	8	3<->0.175	750	10	1 ; 0 ; 0.1 ; 0	7.5
RE32	8	3<->0.175	750	10	0 ; 1 ; 0.1 ; 0	7.5
RE4	8	10<->0.00316	750	10	1 ; 0 ; 0.1 ; 0	1
RE42	8	10<->0.00316	750	0	1 ; 0 ; 0.1 ; 0	2.5

TABLE 2 – Les protocoles Replica Exchange

1.3 Les protocoles Heuristic

Nom	nombre de cycles
h	110000
h-	1100

TABLE 3 – Les protocoles Heuristic

	h	MC3	MC43	RE1	RE2	RE5	RE3	RE4
1A81	20 :19 :08	8 :29 :23	9 :41 :15	4 :14 :08	2 :31 :33	4 :12 :24	3 :39 :51	4 :49 :59
1ABO	4 :46 :51	3 :09 :21	3 :16 :33	2 :58 :01	1 :27 :50	3 :06 :43	2 :02 :08	1 :50 :16
1BM2	17 :57 :45	8 :08 :43	8 :38 :39	5 :04 :51	3 :05 :15	4 :10 :46	3 :31 :43	3 :09 :45
1CKA	5 :51 :19	3 :15 :59	3 :24 :43	2 :25 :53	1 :27 :11	2 :32 :08	2 :05 :03	2 :06 :42
1G9O	12 :15 :20	5 :51 :24	6 :15 :08	3 :44 :15	2 :12 :23	4 :29 :59	3 :05 :30	2 :46 :02
1M61	18 :12 :19	7 :41 :35	8 :07 :18	3 :55 :23	2 :20 :05	4 :07 :41	3 :14 :59	3 :30 :48
1O4C	21 :42 :26	9 :08 :38	9 :57 :44	4 :44 :12	2 :46 :47	4 :27 :51	4 :34 :02	3 :29 :06
1R6J	12 :15 :27	5 :32 :21	5 :59 :11	3 :25 :07	2 :07 :39	3 :27 :18	3 :34 :57	2 :45 :59
2BYG	15 :08 :07	6 :28 :44	6 :56 :15	3 :50 :38	2 :52 :42	4 :49 :02	3 :58 :10	2 :56 :50

TABLE 4 – les temps de calculs (hh :mm :ss) pour tous les résidus actifs

Protéine	h	MC3	MC43	RE1	RE2	RE5	RE3	RE32	RE4
1A81	-521	-538	-522	-525	-520	-520	-514	-512	-518
1ABO	-272	-274	-268	-273	-269	-273	-268	-271	-272
1BM2	-484	-500	-486	-488	-481	-489	-478	-476	-486
1CKA	-252	-258	-249	-259	-251	-251	-247	-246	-249
1G9O	-428	-435	-428	-429	-421	-430	-428	-425	-428
1M61	-480	-493	-479	-483	-480	-481	-480	-480	-480
1O4C	-535	-545	-531	-536	-529	-536	-527	-524	-532
1R6J	-407	-419	-414	-415	-409	-411	-409	-408	-414
2BYG	-457	-469	-454	-461	-456	-460	-456	-454	-462

TABLE 5 – les meilleurs énergies pour tous les résidus actifs

Protéine	GMEC	H-	MC0	MC4-
1A81	-585.1365	0	.2547	0
1ABO	-320.1798	0	0	0
1BM2	-553.5532	0	.0564	.0121
1CKA	-319.2787	0	0	0
1G9O	-481.1175	0	.1394	0
1M61	-555.9140	0	0	0
1O4C	-591.2115	0	0	.1250
1R6J	-454.9340	0	0	0
2BYG	-507.0165	0	0	0

TABLE 6 – l'énergie du GMEC et la différence avec les autres protocoles.Tous les résidus sont gélés

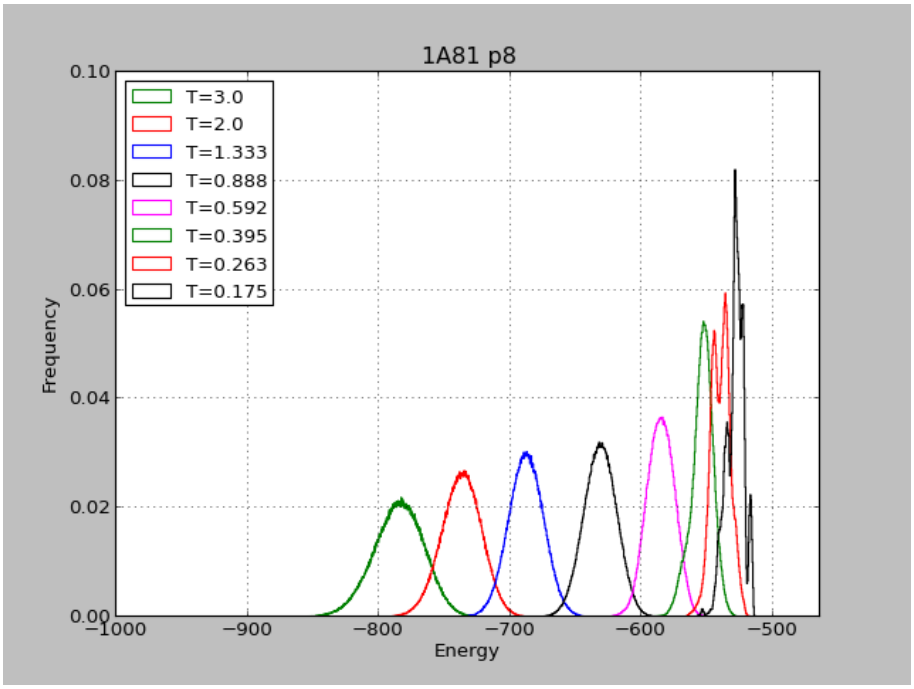

FIGURE 1 – Distribution des énergies selon la température (protocole RE3).

2 Tous les résidus actifs

2.1 Les temps de calculs

2.2 Les meilleures énergies

3 Avec des résidus gélés

3.1 Séquence native

3.2 Séquence native

Protéine	GMEC	H-	MC0	MC4-
1A81	-585.1365	0	.2547	0
1ABO	-320.1798	0	0	0
1BM2	-553.5532	0	.0564	.0121
1CKA	-319.2787	0	0	0
1G9O	-481.1175	0	.1394	0
1M61	-555.9140	0	0	0
1O4C	-591.2115	0	0	.1250
1R6J	-454.9340	0	0	0
2BYG	-507.0165	0	0	0

TABLE 7 – l'énergie du GMEC et la différence avec les autres protocoles.Tous les résidus sont gélés

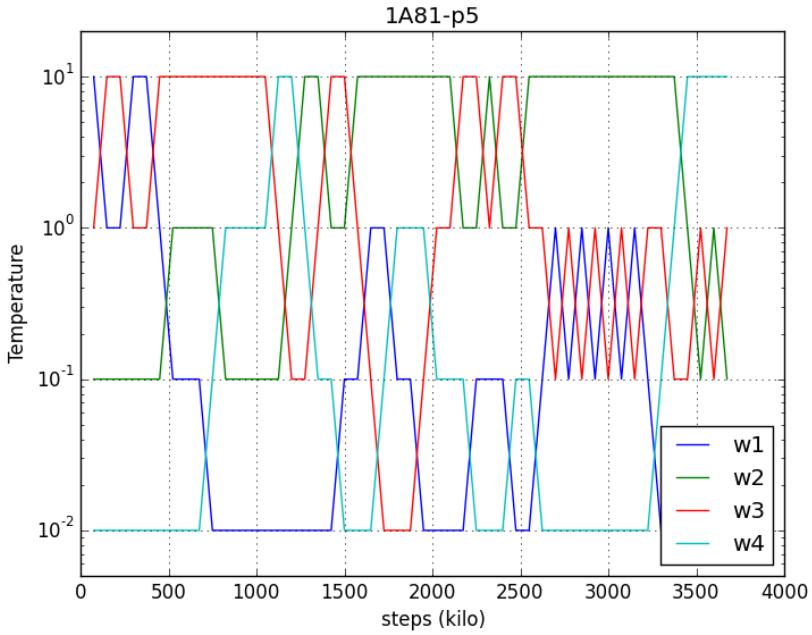

FIGURE 2 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

3.3 Une position active

Position	GMEC	MC4-
14	-584.4693	.0405
39	-584.7378	.0111
55	-584.0477	.0012
60	-583.7763	.0140
66	-592.3835	.0347
70	-583.8950	.0348
71	-588.5916	.0247
76	-583.3815	.0248
79	-582.8485	.0406
86	-584.1412	.0248
101	-583.8406	.0248
105	-583.0197	.0248
107	-582.2241	.0248

TABLE 8 – Liste des echecs pour 1A81

Position	GMEC	MC4-
2	-553.3134	.0040
3	-553.5532	.0121
5	-553.0932	.0179
6	-553.5532	.0121
8	-556.1917	.0148
10	-551.4990	.0149
11	-551.8859	.0149
12	-550.8152	.0148
13	-553.4829	.0451
14	-553.5532	.0121
15	-553.5532	.0121
17	-553.5532	.0121
18	-553.0880	.0121
19	-553.5532	.0270
20	-553.0003	.0121
21	-553.5532	.0121
22	-553.1769	.0121
29	-553.5532	.0121
34	-553.5532	.0270
36	-555.3358	.0317
37	-553.5532	.0121
41	-553.5076	.0121
46	-552.9056	.0149
49	-553.5532	.0121
51	-553.5532	.0179
55	-551.8384	.0121
56	-553.5532	.0121
57	-561.0695	.0121
58	-553.5532	.0121
62	-553.5532	.0121
65	-553.5532	.0121
66	-551.2026	.0179
68	-552.6182	.0148
70	-553.5532	.0121
72	-552.2724	.0121
73	-553.5532	.0121
75	-553.5532	.0179
77	-553.0234	.0466
80	-553.5532	.0121
81	-553.5532	.0121
82	-548.0641	.0121
83	-553.5532	.0121
85	-550.1884	.0122
86	-552.7375	.0148
87	-550.6139	.0121
90	-552.8601	.0009
91	-553.5532	.0121
92	-553.5532	.0121
93	-553.2772	.0148
94	-553.3207	.0251
96	-553.5532	.0121

TABLE 9 – Liste des echecs pour 1BM2

Position	GMEC	MC4-
17	-316.1693	.0109

TABLE 10 – Liste des echecs pour 1CKA

Position	GMEC	MC4
58	-561.9469	.0138

TABLE 11 – Liste des echecs pour 1M61

3.4 Cinq positions actives

3.5 Dix positions actives

3.6 Vingt positions actives

3.7 Trente positions actives

Position	GMEC	MC4-
1	-591.2115	.1380
2	-591.2115	.1250
3	-591.2115	.1250
4	-590.7216	.0319
5	-590.5458	.1071
6	-591.2115	.1521
7	-590.7923	.1429
8	-591.2115	.1250
9	-591.2115	.1728
10	-591.2115	.2572
11	-589.9443	.2489
12	-591.1022	.1137
13	-589.9867	.0535
14	-591.2115	.1250
15	-589.4899	.0436
16	-591.2115	.1521
17	-590.4460	.0557
18	-589.0053	.1366
19	-590.7580	.0348
20	-591.2115	.1250
21	-591.2115	.1600
22	-591.2115	.1250
23	-590.5249	.1530
24	-590.7262	.0630
25	-591.2115	.1250
26	-591.2115	.1250
27	-590.8058	.1194
28	-591.2115	.1250
29	-591.2115	.1571
30	-590.5207	.0221
31	-590.5507	.0530
32	-591.2115	.1571
33	-591.2115	.1234
34	-590.7486	.1258
35	-591.2115	.0378
36	-589.1510	.0974
37	-591.0133	.0941
38	-589.2126	.2743
39	-589.0387	.1890
40	-590.8793	.0883
41	-589.4209	.0409
42	-591.2115	.1250
43	-587.9420	.1315
44	-589.8470	.0595
45	-591.2115	.1712
46	-588.8346	.2668
47	-589.9117	.2773
48	-588.6520	.2625
49	-591.2115	.2120
50	-590.6561	.0807
51	-591.1249	.2986
52	-589.7127	.2734

Position	GMEC	MC4-
4	-453.4484	.0155
20	-452.6464	.0114
32	-454.9340	.0092
68	-454.4856	.0060
73	-454.7809	.0155
77	-454.1344	.0155
79	-453.4729	.0155

TABLE 13 – Liste des echecs pour 1R6J

Position	GMEC	MC4-
1	-505.2910	.0132
3	-506.7960	.0254
4	-505.5800	.0023
5	-506.8732	.0948
49	-505.5183	.0135
59	-507.0165	.0100
85	-506.6217	.0101
88	-505.2286	.0097
95	-506.3195	.0131

TABLE 14 – Liste des echecs pour 2BYG

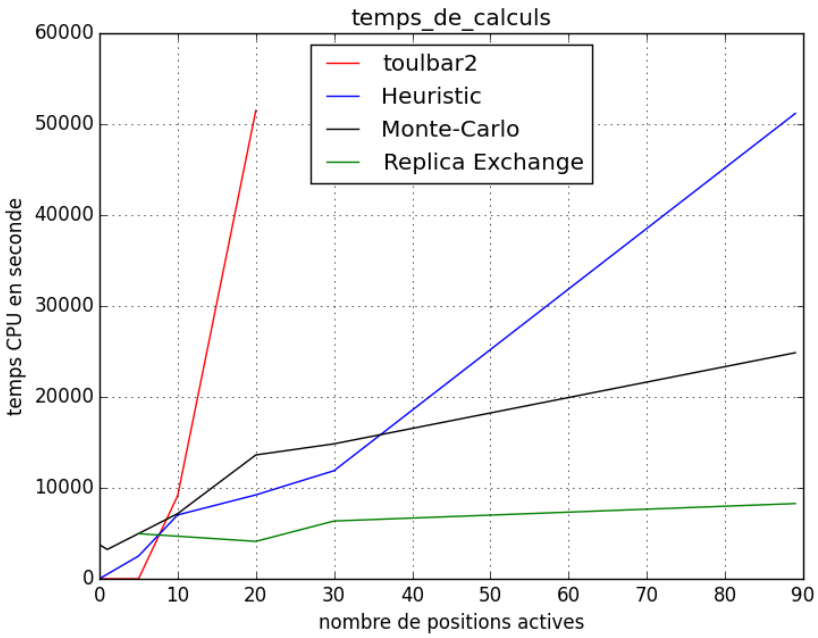

FIGURE 3 – Temps de calculs selon le nombre de positions actives.

Protéine	GMEC	H	MC4
1A81 1	-579.3989	0	0
1A81 2	-575.2254	0	0
1A81 3	-582.7452	0	0
1A81 4	-569.9383	0	5.3443
1A81 5	-591.8143	0	0
1ABO 1	-315.4497	0	0
1ABO 2	-316.6637	0	0
1ABO 3	-307.4824	0	0
1ABO 4	-313.7710	0	0
1ABO 5	-313.5695	0	0
1BM2 1	-548.2341	0	0
1BM2 2	-554.8135	0	0
1BM2 3	-557.8629	0	0
1BM2 4	-544.9791	0	0
1BM2 5	-550.2956	0	.0121
1CKA 1	-315.0859	0	0
1CKA 2	-309.7692	0	0
1CKA 3	-317.3820	0	0
1CKA 4	-314.8550	0	0
1CKA 5	-312.0405	-.0001	-.0001
1G9O 1	-469.9540	0	0
1G9O 2	-476.4094	0	0
1G9O 3	-479.7190	0	0
1G9O 4	-478.9513	0	0
1G9O 5	-480.7260	0	0
1M61 1	-557.6647	0	0
1M61 2	-546.9587	0	0
1M61 3	-553.0731	0	0
1M61 4	-555.0885	0	0
1M61 5	-554.6356	0	0
1O4C 1	-584.4267	0	.0655
1O4C 2	-584.8989	0	.1437
1O4C 3	-588.4971	0	.1164
1O4C 4	-587.7129	0	.1400
1O4C 5	-587.6514	0	.1168
1R6J 1	-444.5018	0	0
1R6J 2	-449.3043	0	.9421
1R6J 3	-453.1139	0	0
1R6J 4	-453.1139	0	0
1R6J 5	-454.9340	0	0
2BYG 1	-500.7946	0	.0150
2BYG 2	-506.2319	0	0
2BYG 3	-506.8744	0	.0131
2BYG 4	-504.5135	0	0
2BYG 5	-506.0052	0	0

TABLE 15 – Liste des echecs pour 2BYG

Protéine	GMEC	H	MC4
1A81 1	-583.9354	0	0
1A81 2	-581.7802	0	0
1A81 3	-587.4392	.0001	.1595
1A81 4	-589.1322	0	.0317
1A81 5	-578.2558	0	.0563
1ABO 1	-309.1670	.0675	.9054
1ABO 2	-308.8387	0	0
1ABO 3	-303.8520	0	0
1ABO 4	-310.0087	0	.0128
1ABO 5	-301.6727	0	0
1BM2 1	-549.8638	0	.0950
1BM2 2	-541.5944	0	0
1BM2 3	-543.7434	0	0
1BM2 4	-549.0453	0	0
1BM2 5	-544.1447	0	.1082
1CKA 1	-305.8477	0	0
1CKA 2	-309.9886	0	0
1CKA 3	-304.6618	0	0
1CKA 4	-302.4894	0	0
1CKA 5	-299.2329	.2859	3.2525
1G9O 1	-466.6764	0	0
1G9O 2	-478.8797	0	0
1G9O 3	-477.2503	.1366	0
1G9O 4	-470.6458	0	0
1G9O 5	-464.8659	0	3.9599
1M61 1	-550.0699	0	.0776
1M61 2	-538.6026	3.5105	4.5062
1M61 3	-552.2673	0	0
1M61 4	-550.0553	0	0
1M61 5	-553.6559	0	.0432
1O4C 1	-587.4665	0	.1121
1O4C 2	-585.8545	0	.1046
1O4C 3	-580.3505	0	.1519
1O4C 4	-587.1548	0	.1545
1O4C 5	-590.2650	0	.1753
1R6J 1	-448.8351	0	2.4022
1R6J 2	-448.4631	0	1.0398
1R6J 3	-450.3950	0	.0106
1R6J 4	-451.7211	0	0
1R6J 5	-450.9943	0	.0162
2BYG 1	-511.3882	-5.7485	-5.7148
2BYG 2	-504.7389	0	0
2BYG 3	-504.3048	0	.0833
2BYG 4	-504.3466	0	.2149
2BYG 5	-491.6095	0	0

TABLE 16 – Résultats 10 positions actives

Protéine	GMEC	H	MC4
1A81 1	-566.9106	0	.3275
1A81 2	-564.6618	.1705	2.4355
1A81 3	-572.9780	0	.4640
1A81 4	-572.9780	.3568	.5088
1A81 5	-572.9780	.3568	.5088
1ABO 1	-299.6592	.1205	1.1159
1ABO 2	no	-298.3854	-298.3854
1ABO 3	no	-298.3854	298.3854
1ABO 4	no	-297.8545	-297.8621
1ABO 5	no	-297.8009	-298.7492
1BM2 1	-526.0936	0	.0619
1BM2 2	no	-525.3588	-525.4313
1BM2 3	-534.3860	.0230	.4763
1BM2 4	no	-526.8307	-529.4190
1BM2 5	-535.3334	.2396	.3746
1CKA 1	-295.8571	0	0
1CKA 2	-295.8571	0	0
1CKA 3	-293.8687	0	0
1CKA 4	no	-293.8687	-293.8687
1CKA 5	no	-293.4203	-293.4203
1G9O 1	no	-451.4604	-452.7129
1G9O 2	no	-453.2474	-453.4651
1G9O 3	no	-453.2474	-453.4651
1G9O 4	no	-456.7331	-456.8786
1G9O 5	no	-456.7331	-456.8786
1M61 1	-528.0700	0	0
1M61 2	-528.7653	0	0
1M61 3	-530.0684	0	0
1M61 4	-534.5248	0	0
1M61 5	-548.0096	0	.2521
1O4C 1	no	-574.3512	-574.0737
1O4C 2	no	-574.8584	-575.0547
1O4C 3	-573.6314	0	.3461
1O4C 4	-575.8667	0	.3640
1O4C 5	no	-573.3479	-573.4610
1R6J 1	-440.7417	0	.2604
1R6J 2	-437.2537	0	.0071
1R6J 3	-439.4335	0	.0537
1R6J 4	-439.4335	0	.0537
1R6J 5	-438.0222	0	.0735
2BYG 1	-496.2991	0	3.1878
2BYG 2	-494.8723	0	.0524
2BYG 3	-494.8723	0	1.3564
2BYG 4	-495.9213	0	.1968
2BYG 5	no	-497.5123	-497.6056

TABLE 17 – Résultats 20 positions actives

Protéine	GMEC	H	MC4
1A81 1	no	-562.9572	-563.5925
1A81 2	no	-570.2620	-570.3198
1A81 3	no	-562.9572	no
1A81 4	no	-559.6145	-559.6450
1A81 5	no	-553.1077	-555.0663
1ABO 1	no	-296.5680	-296.5680
1ABO 2	no	-294.8500	-294.8500
1ABO 3	no	-295.2689	-295.5319
1ABO 4	no	-296.5680	-296.5680
1ABO 5	no	-296.5680	-296.5680
1BM2 1	no	-529.6542	-530.4102
1BM2 2	no	-529.6542	-596.2084
1BM2 3	no	-529.9719	-531.1130
1BM2 4	no	-529.9719	-531.1130
1BM2 5	no	-527.3240	-528.8384
1CKA 1	no	-293.4203	-293.4203
1CKA 2	no	-293.4203	-293.4203
1CKA 3	no	-291.9243	-291.9243
1CKA 4	no	-293.4203	-293.4203
1CKA 5	no	-293.2709	-293.2709
1G9O 1	no	-449.0890	-450.6832
1G9O 2	no	-452.6676	-452.9802
1G9O 3	no	-450.0341	-451.6008
1G9O 4	no	-453.9682	-455.3966
1G9O 5	no	-447.5800	-453.5895
1M61 1	no	-523.9418	-523.9321
1M61 2	no	-531.3717	-533.2466
1M61 3	no	-527.2659	-527.2813
1M61 4	no	-530.2666	-530.2666
1M61 5	no	-522.5696	-522.5696
1O4C 1	no	-571.4882	-571.8317
1O4C 2	no	-570.1458	-570.2253
1O4C 3	no	-569.9777	-570.1566
1O4C 4	no	-568.9839	-569.0262
1O4C 5	no	-569.9777	-570.1566
1R6J 1	no	-435.4258	-435.4504
1R6J 2	no	-435.0087	-435.1044
1R6J 3	no	-439.8187	-439.8627
1R6J 4	no	-435.0087	-435.1044
1R6J 5	no	-435.0087	-435.1044
2BYG 1	no	-492.6879	-492.8471
2BYG 2	no	-492.3568	-492.5070
2BYG 3	no	-492.6879	-492.8471
2BYG 4	no	-492.6879	-492.8471
2BYG 5	no	-492.6879	-492.8471

TABLE 18 – Résultats 30 positions actives