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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

1.4 Les temps de calcul

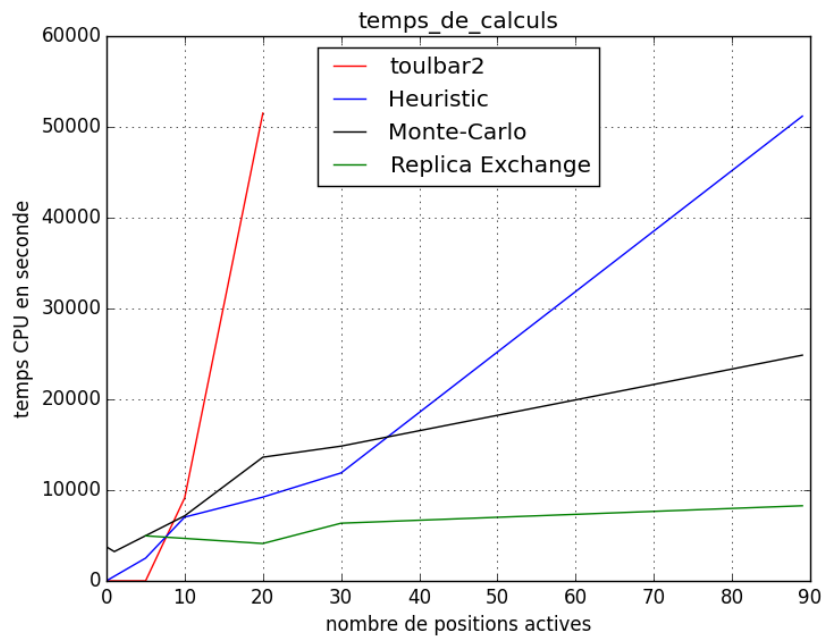


FIGURE 1 – Temps d’occupation du processeur selon le nombre de positions actives.

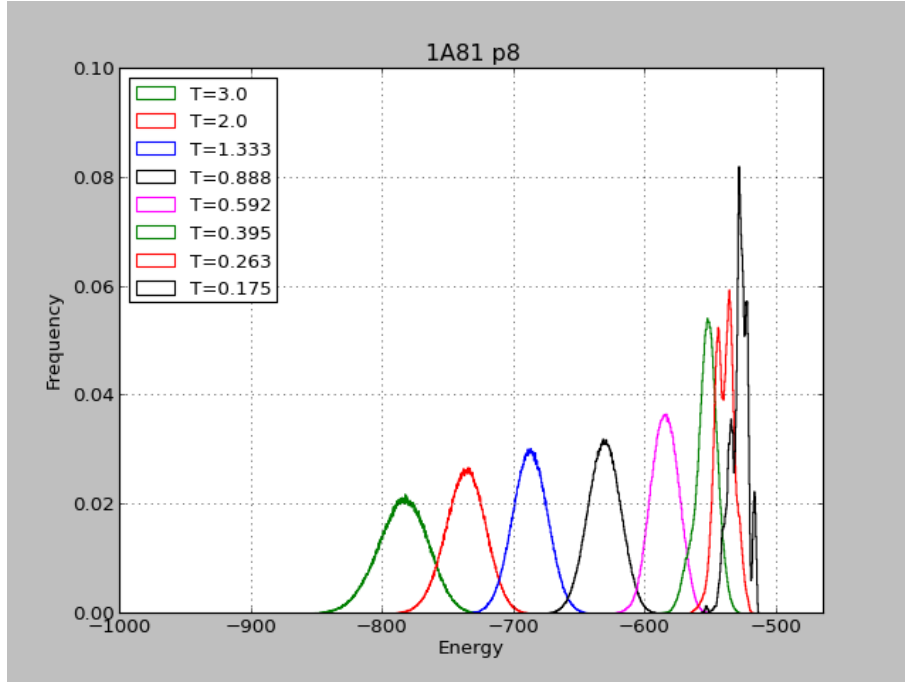


FIGURE 2 – Distribution des énergies selon la température (protocole RE3).

2 Tous les résidus actifs

2.1 Les meilleures énergies

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 4 – les meilleures énergies pour tous les résidus actifs

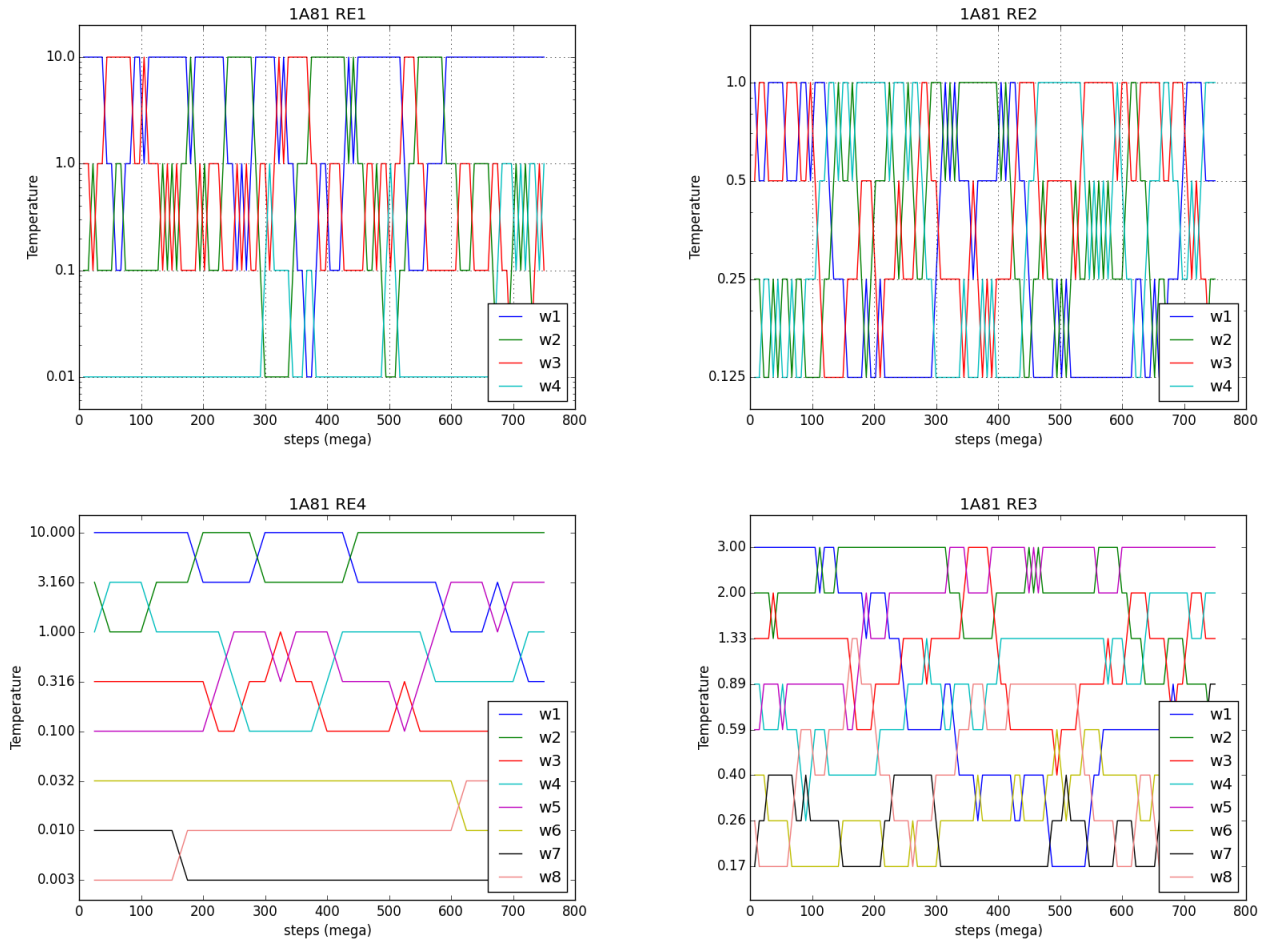


FIGURE 3 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

3 Avec des résidus gelés

3.1 Séquence native

3.2 Une position active

3.3 Cinq positions actives

3.4 Dix positions actives

3.5 Vingt positions actives

3.6 Trente positions actives

3.7 Etude au voisinage de GMECs

Protéine	GMEC	H-	MC0	MC4-
1A81	-585.1365	0	-0.2547	0
1ABO	-320.1798	0	0	0
1BM2	-553.5532	0	-0.0564	-0.0121
1CKA	-319.2787	0	0	0
1G9O	-481.1175	0	-0.1394	0
1M61	-555.9140	0	0	0
1O4C	-591.2115	0	0	-0.1250
1R6J	-454.9340	0	0	0
2BYG	-507.0165	0	0	0

TABLE 5 – L'énergie du GMEC et la différence avec les autres protocoles. Tous les résidus sont gelés

Position	GMEC	MC4-
14	-584.4693	-0.0405
39	-584.7378	-0.0111
55	-584.0477	-0.0012
60	-583.7763	-0.0140
66	-592.3835	-0.0347
70	-583.8950	-0.0348
71	-588.5916	-0.0247
76	-583.3815	-0.0248
79	-582.8485	-0.0406
86	-584.1412	-0.0248
101	-583.8406	-0.0248
105	-583.0197	-0.0248
107	-582.2241	-0.0248

TABLE 6 – Liste des échecs pour 1A81

Position	GMEC	MC4-
2	-553.3134	-0.0040
3	-553.5532	-0.0121
5	-553.0932	-0.0179
6	-553.5532	-0.0121
8	-556.1917	-0.0148
10	-551.4990	-0.0149
11	-551.8859	-0.0149
12	-550.8152	-0.0148
13	-553.4829	-0.0451
14	-553.5532	-0.0121
15	-553.5532	-0.0121
17	-553.5532	-0.0121
18	-553.0880	-0.0121
19	-553.5532	-0.0270
20	-553.0003	-0.0121
21	-553.5532	-0.0121
22	-553.1769	-0.0121
29	-553.5532	-0.0121
34	-553.5532	-0.0270
36	-555.3358	-0.0317
37	-553.5532	-0.0121
41	-553.5076	-0.0121
46	-552.9056	-0.0149
49	-553.5532	-0.0121
51	-553.5532	-0.0179
55	-551.8384	-0.0121
56	-553.5532	-0.0121
57	-561.0695	-0.0121
58	-553.5532	-0.0121
62	-553.5532	-0.0121
65	-553.5532	-0.0121
66	-551.2026	-0.0179
68	-552.6182	-0.0148
70	-553.5532	-0.0121
72	-552.2724	-0.0121
73	-553.5532	-0.0121
75	-553.5532	-0.0179
77	-553.0234	-0.0466
80	-553.5532	-0.0121
81	-553.5532	-0.0121
82	-548.0641	-0.0121
83	-553.5532	-0.0121
85	-550.1884	-0.0122
86	-552.7375	-0.0148
87	-550.6139	-0.0121
90	-552.8601	-0.0009
91	-553.5532	-0.0121
92	-553.5532	-0.0121
93	-553.2772	-0.0148
94	-553.3207	-0.0251
96	-553.5532	-0.0121

TABLE 7 – Liste des échecs pour 1BM2

Position	GMEC	MC4-
17	-316.1693	-0.0109

TABLE 8 – Liste des échecs pour 1CKA

Position	GMEC	MC4
58	-561.9469	-0.0138

TABLE 9 – Liste des échecs pour 1M61

Position	GMEC	MC4-
1	-591.2115	-0.1380
2	-591.2115	-0.1250
3	-591.2115	-0.1250
4	-590.7216	-0.0319
5	-590.5458	-0.1071
6	-591.2115	-0.1521
7	-590.7923	-0.1429
8	-591.2115	-0.1250
9	-591.2115	-0.1728
10	-591.2115	-0.2572
11	-589.9443	-0.2489
12	-591.1022	-0.1137
13	-589.9867	-0.0535
14	-591.2115	-0.1250
15	-589.4899	-0.0436
16	-591.2115	-0.1521
17	-590.4460	-0.0557
18	-589.0053	-0.1366
19	-590.7580	-0.0348
20	-591.2115	-0.1250
21	-591.2115	-0.1600
22	-591.2115	-0.1250
23	-590.5249	-0.1530
24	-590.7262	-0.0630
25	-591.2115	-0.1250
26	-591.2115	-0.1250
27	-590.8058	-0.1194
28	-591.2115	-0.1250
29	-591.2115	-0.1571
30	-590.5207	-0.0221
31	-590.5507	-0.0530
32	-591.2115	-0.1571
33	-591.2115	-0.1234
34	-590.7486	-0.1258
35	-591.2115	-0.0378
36	-589.1510	-0.0974
37	-591.0133	-0.0941
38	-589.2126	-0.2743
39	-589.0387	-0.1890
40	-590.8793	-0.0883
41	-589.4209	-0.0409
42	-591.2115	-0.1250
43	-587.9420	-0.1315
44	-589.8470	-0.0595
45	-591.2115	-0.1712
46	-588.8346	-0.2668
47	-589.9117	-0.2773
48	-588.6520	-0.2625
49	-591.2115	-0.2120
50	-590.6561	-0.0807
51	-591.1249	-0.2986
52	-589.7127	-0.2734
53	-590.7224	-0.2012

Position	GMEC	MC4-
4	-453.4484	-0.0155
20	-452.6464	-0.0114
32	-454.9340	-0.0092
68	-454.4856	-0.0060
73	-454.7809	-0.0155
77	-454.1344	-0.0155
79	-453.4729	-0.0155

TABLE 11 – Liste des échecs pour 1R6J

Position	GMEC	MC4-
1	-505.2910	-0.0132
3	-506.7960	-0.0254
4	-505.5800	-0.0023
5	-506.8732	-0.0948
49	-505.5183	-0.0135
59	-507.0165	-0.0100
85	-506.6217	-0.0101
88	-505.2286	-0.0097
95	-506.3195	-0.0131

TABLE 12 – Liste des échecs pour 2BYG

Protéine	GMEC	H	MC4	RE3
1A81 1	-579.3989	0	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	-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	-0.0001	-0.0001	
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	-0.0655	
1O4C 2	-584.8989	0	-0.1437	
1O4C 3	-588.4971	0	-0.1164	
1O4C 4	-587.7129	0	-0.1400	
1O4C 5	-587.6514	0	-0.1168	
1R6J 1	-444.5018	0	0	0
1R6J 2	-449.3043	0	-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	-0.0150	
2BYG 2	-506.2319	0	0	
2BYG 3	-506.8744	0	-0.0131	
2BYG 4	-504.5135	0	0	
2BYG 5	-506.0052	0	0	

TABLE 13 – Résultats 5 position actives

Protéine	GMEC	H	MC4	RE32
1A81 1	-583.9354	0	0	0
1A81 2	-581.7802	0	0	
1A81 3	-587.4392	-0.0001	-0.1595	
1A81 4	-589.1322	0	-0.0317	
1A81 5	-578.2558	0	-0.0563	
1ABO 1	-309.1670	-0.0675	-0.9054	
1ABO 2	-308.8387	0	0	
1ABO 3	-303.8520	0	0	
1ABO 4	-310.0087	0	-0.0128	
1ABO 5	-301.6727	0	0	
1BM2 1	-549.8638	0	-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	-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	-0.2859	-3.2525	
1G9O 1	-466.6764	0	0	
1G9O 2	-478.8797	0	0	
1G9O 3	-477.2503	-0.1366	0	
1G9O 4	-470.6458	0	0	
1G9O 5	-464.8659	0	-3.9599	
1M61 1	-550.0699	0	-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	-0.0432	
1O4C 1	-587.4665	0	-0.1121	
1O4C 2	-585.8545	0	-0.1046	
1O4C 3	-580.3505	0	-0.1519	
1O4C 4	-587.1548	0	-0.1545	
1O4C 5	-590.2650	0	-0.1753	
1R6J 1	-448.8351	0	-2.4022	-2.3986
1R6J 2	-448.4631	0	-1.0398	
1R6J 3	-450.3950	0	-0.0106	
1R6J 4	-451.7211	0	0	
1R6J 5	-450.9943	0	-0.0162	
2BYG 1	-511.3882	0	-0.0337	
2BYG 2	-504.7389	0	0	
2BYG 3	-504.3048	0	-0.0833	
2BYG 4	-504.3466	0	-0.2149	
2BYG 5	-491.6095	0	0	

TABLE 14 – Résultats 10 positions actives

Protéine	GMEC	H	MC4	RE32
1A81 1	-566.9106	0	-0.3275	-1.0069
1A81 2	-564.6618	-0.1705	-2.4355	
1A81 3	-572.9780	0	-0.4640	
1A81 4	-570.3480	-0.3568	-0.5128	
1A81 5	-571.2480	-0.7658	-0.5088	
1ABO 1	-299.6592	-0.1205	-1.1159	-0.2153
1ABO 2	no	-298.3854	0	
1ABO 3	no	-298.3854	0	
1ABO 4	no	-297.8545	-0.0076	
1ABO 5	no	-297.8009	-0.9483	
1BM2 1	-526.0936	0	-0.0619	
1BM2 2	no	-525.3588	-0.0725	-0.0789
1BM2 3	-534.3860	-0.0230	-0.4763	
1BM2 4	no	-526.8307	-2.5883	
1BM2 5	-535.3334	-0.2396	-0.3746	
1CKA 1	-295.6311	0	0	
1CKA 2	-295.8571	0	0	-1.2525
1CKA 3	-293.8687	0	0	
1CKA 4	no	-293.8687	0	
1CKA 5	no	-293.4203	0	
1G9O 1	no	-451.4604	-1.2525	
1G9O 2	no	-453.2355	-0.2487	
1G9O 3	no	-453.2474	-0.2177	
1G9O 4	no	-456.3751	-0.2275	
1G9O 5	no	-456.7331	-0.1455	
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	-0.2521	
1O4C 1	no	-0.2775	-574.0737	
1O4C 2	no	-574.8584	-0.1963	
1O4C 3	-573.6314	0	-0.3461	
1O4C 4	-575.8667	0	-0.3640	
1O4C 5	no	-573.3479	-0.1141	
1R6J 1	-440.7417	0	-0.2604	
1R6J 2	-437.2537	0	-0.0071	
1R6J 3	-439.4335	0	-0.0537	
1R6J 4	-439.9135	0	-0.0537	
1R6J 5	-438.0222	0	-0.0735	
2BYG 1	-496.2991	0	-3.1878	-0.0257
2BYG 2	-494.8723	0	-0.0524	-0.0826
2BYG 3	-494.8723	0	-1.3564	
2BYG 4	-495.9213	0	-0.1968	
2BYG 5	no	-497.5123	-0.0933	

TABLE 15 – Résultats 20 positions actives

Protéine	GMEC	H	MC4	RE32	
1A81 1	no	-562.9572	-0.6353		
1A81 2	no	-570.2620	-0.0578		
1A81 3	no	-562.9572	-0.3580		
1A81 4	no	-559.6145	-0.0305		
1A81 5	no	-553.1077	-1.9586	-0.5791	
1ABO 1	no	-296.5680	0		
1ABO 2	no	-294.8500	0		
1ABO 3	no	-295.2689	-0.2630		
1ABO 4	no	-296.5680	0		
1ABO 5	no	-296.1598	0		
1BM2 1	no	-529.6542	-0.7560		
1BM2 2	no	-529.7536	-0.7528		
1BM2 3	no	-529.9719	-1.1411	-1.1319	
1BM2 4	no	-528.3456	-1.1411	-1.1319	
1BM2 5	no	-527.3240	-1.5144	-1.1937	
1CKA 1	no	-293.8208	0		
1CKA 2	no	-293.4203	0		
1CKA 3	no	-291.9243	0		
1CKA 4	no	-293.4203	0		
1CKA 5	no	-293.2709	0		
1G9O 1	no	-449.0890	-1.5942	0	
1G9O 2	no	-452.6676	-0.3126		
1G9O 3	no	-450.0341	-1.5667	-1.5852	-1.5235
1G9O 4	no	-453.9682	-1.4284	-1.6390	-1.6202
1G9O 5	no	-1.4509	-7.4604	-446.1291	
1M61 1	no	-0.0097	-523.9321	0	
1M61 2	no	-531.3717	-1.8749	-0.0083	
1M61 3	no	-527.2659	-0.0154		
1M61 4	no	-530.2666	0		
1M61 5	no	-522.5696	0		
1O4C 1	no	-571.4882	-0.3435		
1O4C 2	no	-570.1458	-0.0795		
1O4C 3	no	-569.9777	-0.1789		
1O4C 4	no	-568.9839	-0.0423		
1O4C 5	no	-569.9471	-0.1892		
1R6J 1	no	-435.4258	-0.0246		
1R6J 2	no	-435.0087	-0.0957		
1R6J 3	no	-439.8187	-0.0440		
1R6J 4	no	-435.0087	-0.0957		
1R6J 5	no	-434.5687	-0.0047		
2BYG 1	no	-492.2456	-0.1592		
2BYG 2	no	-490.3568	-0.1582		
2BYG 3	no	-492.5667	-0.2572		
2BYG 4	no	-491.6879	-0.1542		
2BYG 5	no	-492.7722	-0.0593		

TABLE 16 – Résultats 30 positions actives

Protéine	nb seq (GMEC + 1)	rang H	rang MC	rang RE
1CKA 3	67668	1	1	1
1CKA 4	4647	1	1	
1CKA 5	255	10	182638	
1G9O 3	435881	24	1	1
1G9O 4	354476	1	1	
1G9O 5	61	1	897112	
1M61 2	261467	1	1	
1M61 3	11199152			
1M61 4	16417603			

TABLE 17 – Résultats 30 positions actives