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1.1 Toulbar2

1.2 l'heuristique

1.3 Le Monte-Carlo

1.4 Le Replica Exchange

2 Les protocoles

2.1 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

2.2 Les protocoles Replica Exchange

2.3 Les protocoles Heuristic

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

Nom	nombre de cycles
h	110000
h-	1100

TABLE 3 – Les protocoles Heuristic

2.4 Les temps de calcul

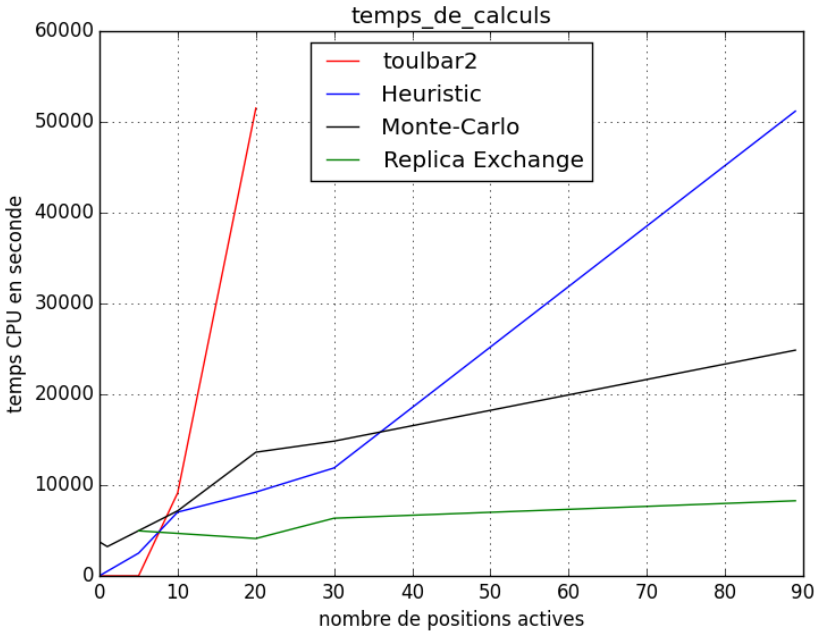

FIGURE 1 – Temps d'occupation du processeur selon le nombre de positions actives.

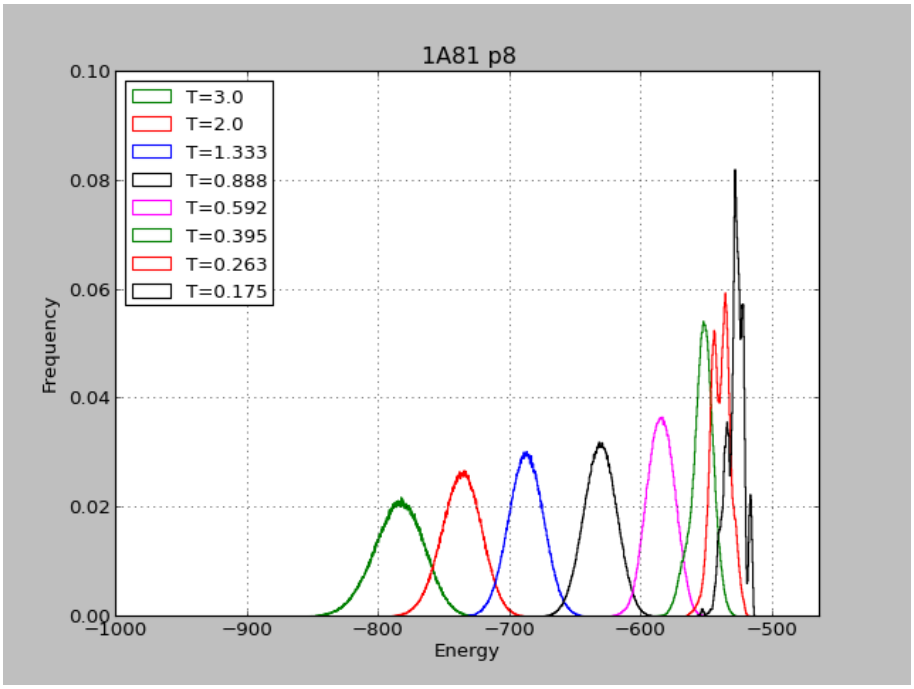

FIGURE 2 – Distribution des énergies selon la température (protocole RE3).

3 Les tests

3.1 Tous les résidus actif

3.1.1 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

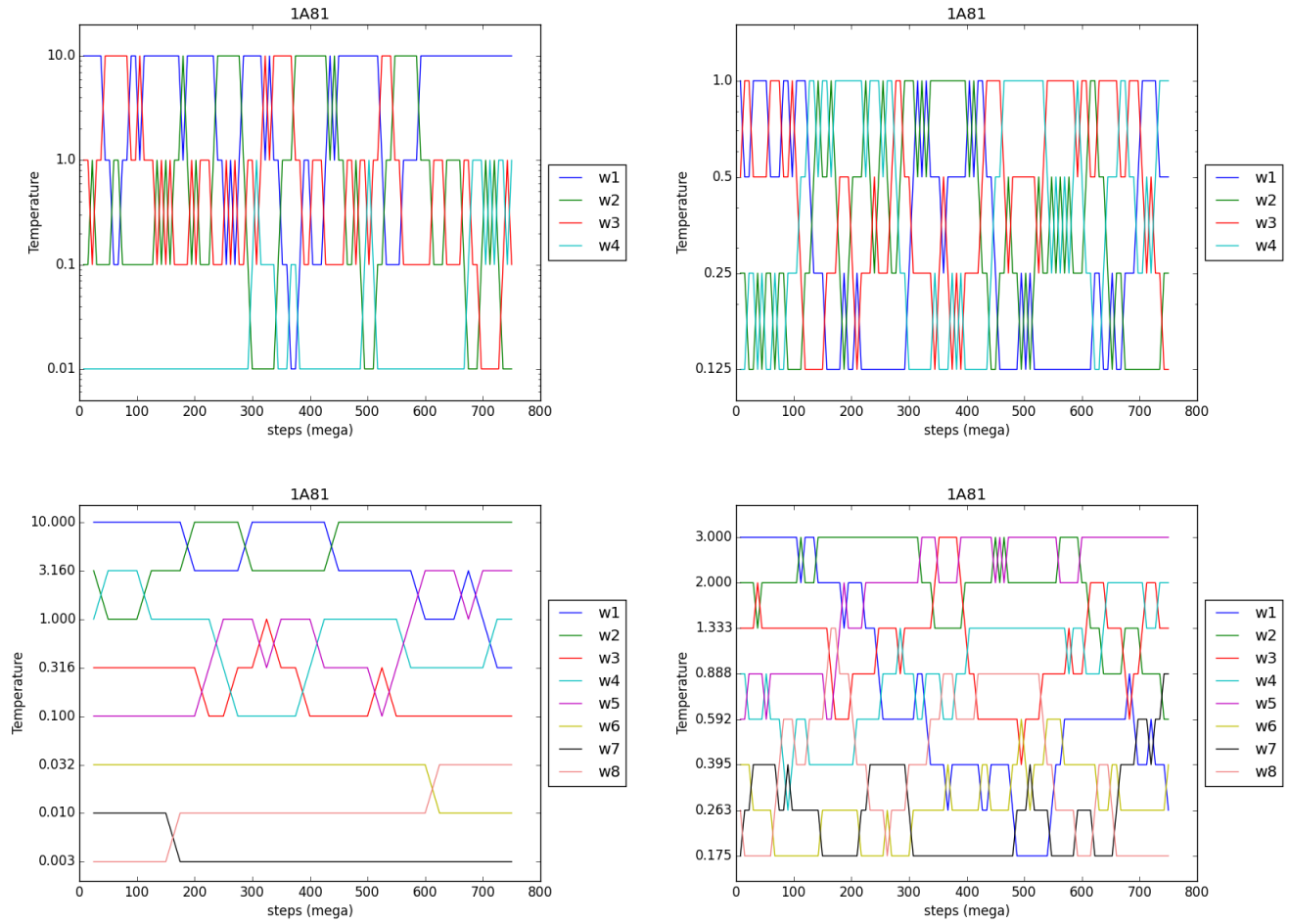

FIGURE 3 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

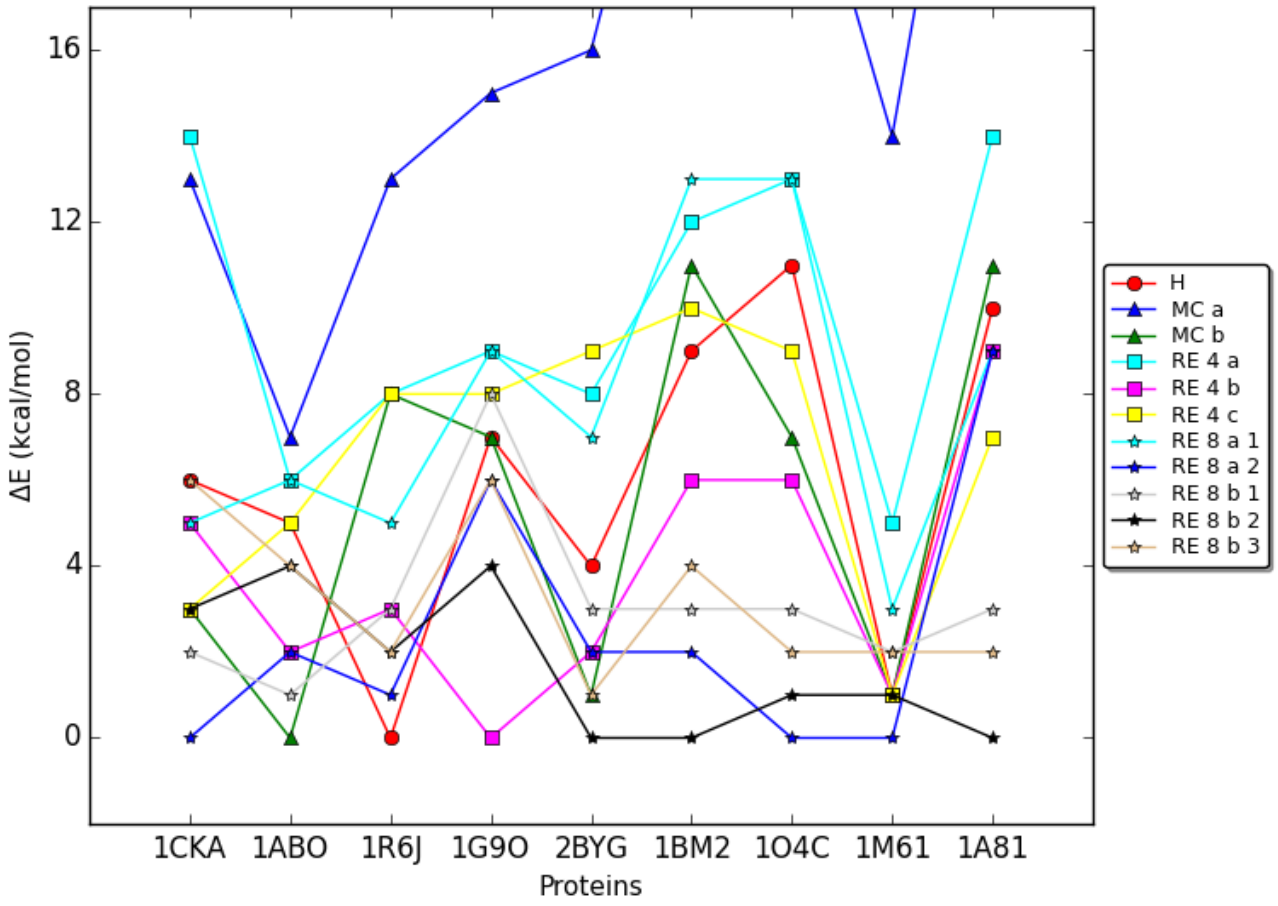

FIGURE 4 – Tous les protocoles.

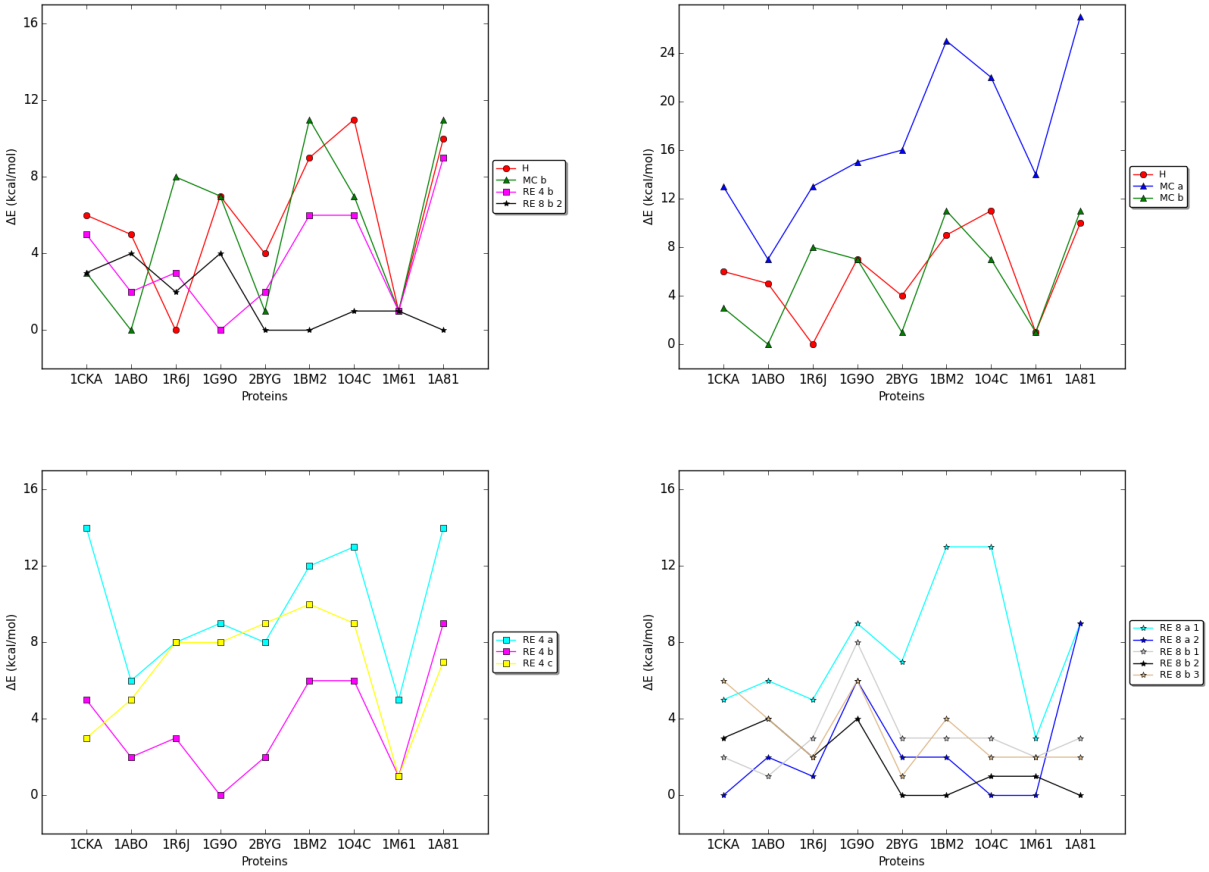

FIGURE 5 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

3.2 Avec des résidus gelés

3.2.1 Séquence native

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

3.2.2 Une position active

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

3.2.3 Cinq positions actives

3.2.4 Dix positions actives

3.2.5 Vingt et trente positions actives

3.3 Etude au voisinnage de GMECs

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	-0.2913

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	
1A81 2	-575.2254	0	0	
1A81 3	-582.7452	0	0	
1A81 4	-569.9383	0	-5.3443	0
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	
1R6J 2	-449.3043	0	-0.9421	0
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	
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	0
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	0.3215
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	no	-505.6397	-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

10 positions actives					20 positions actives			
Protéine	GMEC	H	MC	RE	GMEC	H	MC	RE
1A81 1	-583.9354	0	0		-566.9106	0	-0.3275	-.3851
1A81 2	-581.7802	0	0		-564.6618	-0.1705	-2.4355	-1.0069
1A81 3	-587.4392	-0.0001	-0.1595		-572.9780	0	-0.4640	-.6186
1A81 4	-589.1322	0	-0.0317		-570.3480	-0.3568	-0.5128	-.6991
1A81 5	-578.2558	0	-0.0563		-571.2480	-0.7658	-0.5088	-.6991
1ABO 1	-309.1670	-0.0675	-0.9054		-299.6592	-0.1205	-1.1159	-0.2153
1ABO 2	-308.8387	0	0		no	-298.3854	0	0
1ABO 3	-303.8520	0	0		no	-298.3854	0	0
1ABO 4	-310.0087	0	-0.0128		no	-297.8545	-0.0076	0
1ABO 5	-301.6727	0	0		no	-297.8009	-0.9483	-.9483
1BM2 1	-549.8638	0	-0.0950		-526.0936	0	-0.0619	-.1584
1BM2 2	-541.5944	0	0		no	-525.3588	-0.0725	-.0143
1BM2 3	-543.7434	0	0		-534.3860	-0.0230	-0.4763	-.2898
1BM2 4	-549.0453	0	0		no	-526.8307	-2.5883	-0.0789
1BM2 5	-544.1447	0	-0.1082		-535.3334	-0.2396	-0.3746	-.3746
1CKA 1	-305.8477	0	0		-295.6311	0	0	0
1CKA 2	-309.9886	0	0		-295.8571	0	0	0
1CKA 3	-304.6618	0	0		-293.8687	0	0	0
1CKA 4	-302.4894	0	0		no	-293.8687	0	0
1CKA 5	-299.2329	-0.2859	-3.2525	0	no	-293.4203	0	0
1G9O 1	-466.6764	0	0		no	-451.4604	-1.2525	-1.2525
1G9O 2	-478.8797	0	0		no	-453.2355	-0.2487	-.1915
1G9O 3	-477.2503	-0.1366	0		no	-453.2474	-0.2177	-.1915
1G9O 4	-470.6458	0	0		no	-456.3751	-0.2275	-.1455
1G9O 5	-464.8659	0	-3.9599		no	-456.7331	-0.1455	-.1455
1M61 1	-550.0699	0	-0.0776		-528.0700	0	0	0
1M61 2	-538.6026	-3.5105	-4.5062	0.3215	-528.7653	0	0	0
1M61 3	-552.2673	0	0		-530.0684	0	0	0
1M61 4	-550.0553	0	0		-534.5248	0	0	0
1M61 5	-553.6559	0	-0.0432		-548.0096	0	-0.2521	-0.1345
1O4C 1	-587.4665	0	-0.1121		no	-.2878	-.0103	-574.0634
1O4C 2	-585.8545	0	-0.1046		no	-574.8584	-0.1963	-.3175
1O4C 3	-580.3505	0	-0.1519		-573.6314	0	-0.3461	-.0997
1O4C 4	-587.1548	0	-0.1545		-575.8667	0	-0.3640	-.1382
1O4C 5	-590.2650	0	-0.1753		no	-573.3479	-0.1141	-.2206
1R6J 1	-448.8351	0	-2.4022	-0.3986	-440.7417	0	-0.2604	-.2002
1R6J 2	-448.4631	0	-1.0398		-437.2537	0	-0.0071	-.0183
1R6J 3	-450.3950	0	-0.0106		-439.4335	0	-0.0537	-.0732
1R6J 4	-451.7211	0	0		-439.9135	0	-0.0537	-.0732
1R6J 5	-450.9943	0	-0.0162		-438.0222	0	-0.0735	-.0244
2BYG 1	no	-505.6397	-0.0337		-496.2991	0	-3.1878	-.0257
2BYG 2	-504.7389	0	0		-494.8723	0	-0.0524	-.0826
2BYG 3	-504.3048	0	-0.0833		-494.8723	0	-1.3564	-.0826
2BYG 4	-504.3466	0	-0.2149		-495.9213	0	-0.1968	-.6022
2BYG 5	-491.6095	0	0		no	-497.5123	-0.0933	-.0386

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

TABLE 15 – Résultats 30 positions actives

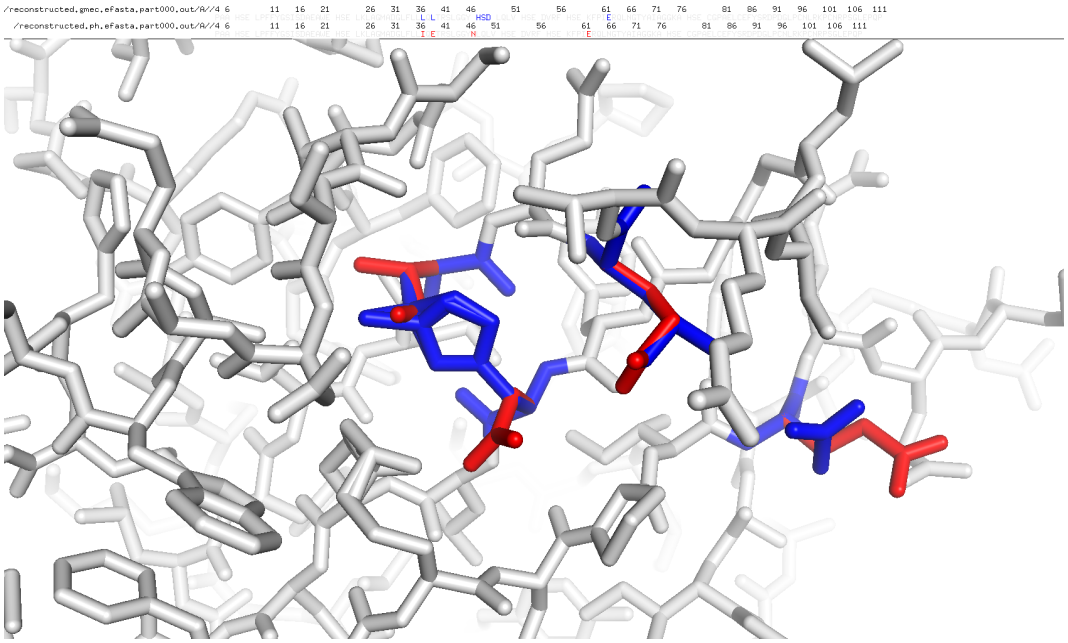

FIGURE 6 – test : 1M61 2, GMEC vs H

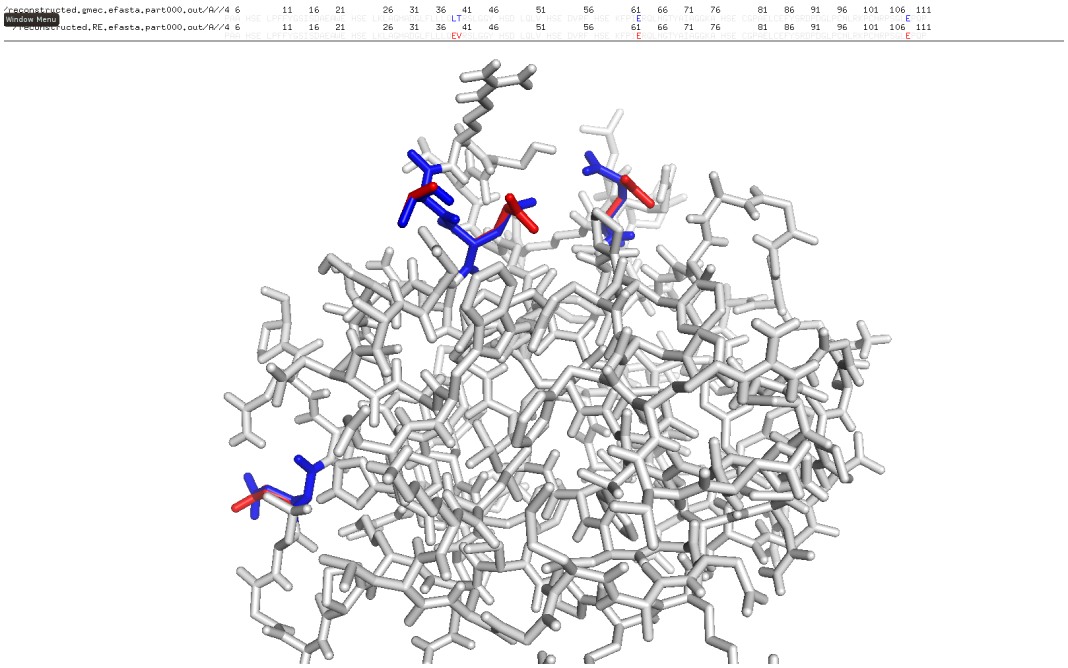

FIGURE 7 – test : 1M61 2, GMEC vs RE

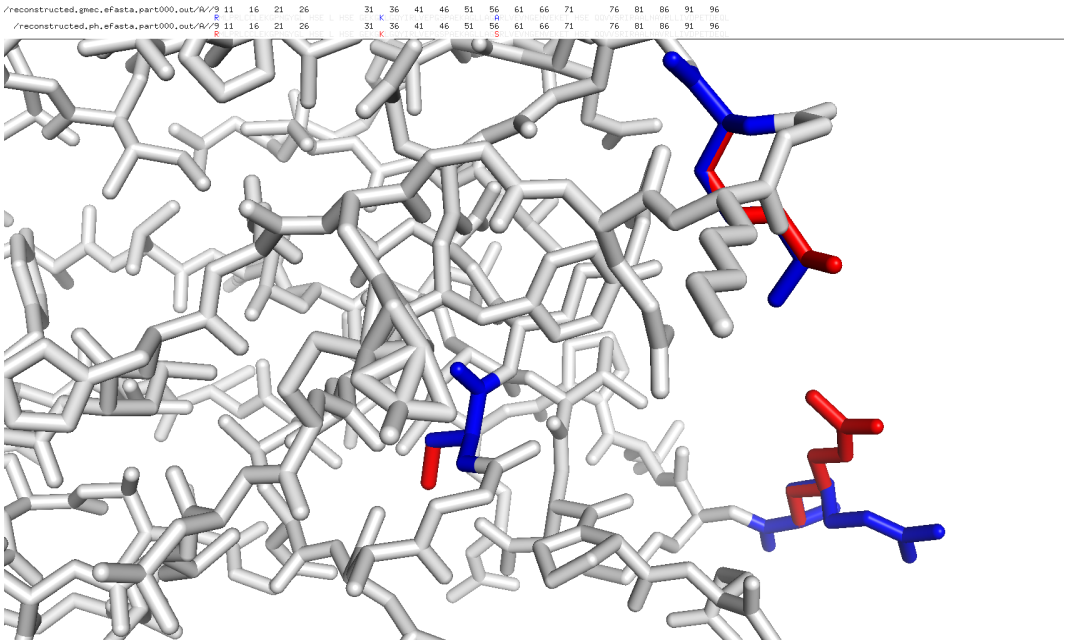

FIGURE 8 – test : 1G9O 3, GMEC vs H

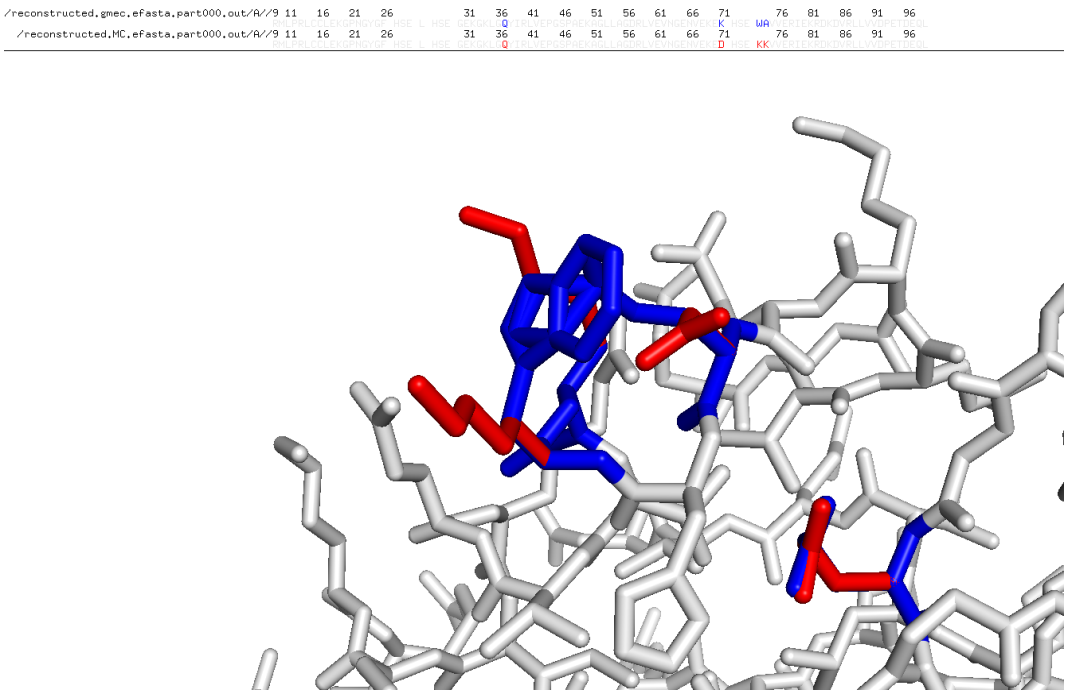

FIGURE 9 – test : 1G9O 5, GMEC vs MC

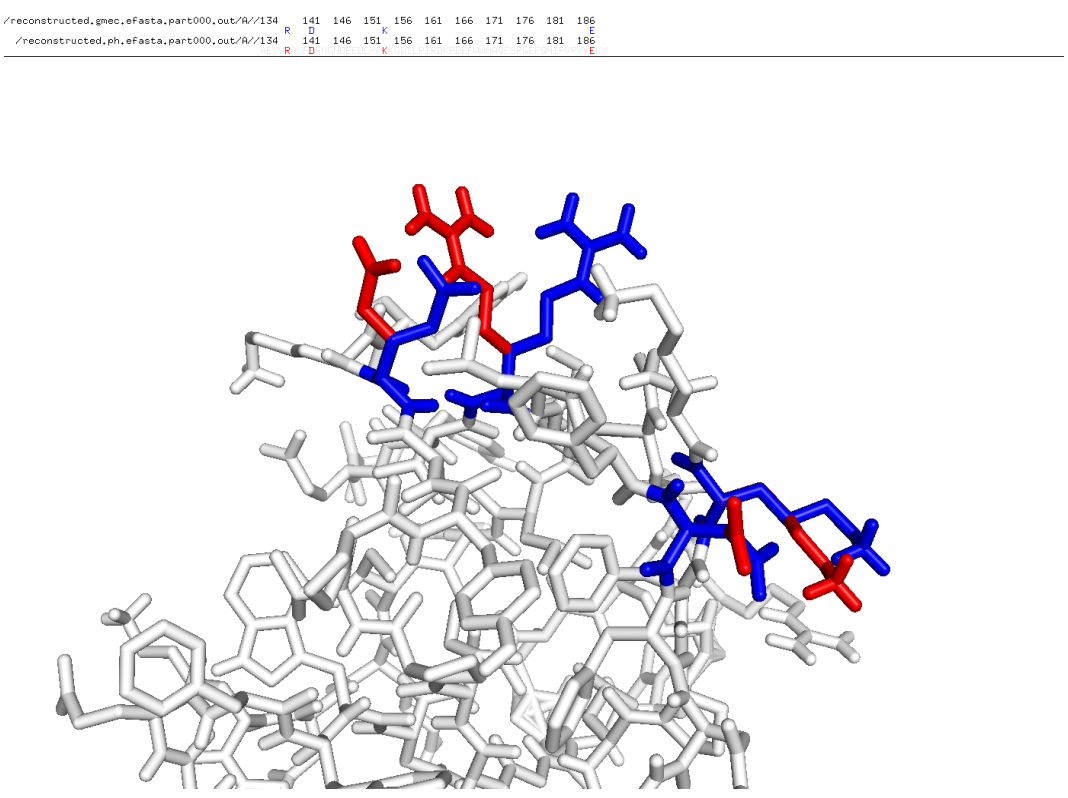

FIGURE 10 – test : 1CKA 5, GMEC vs H

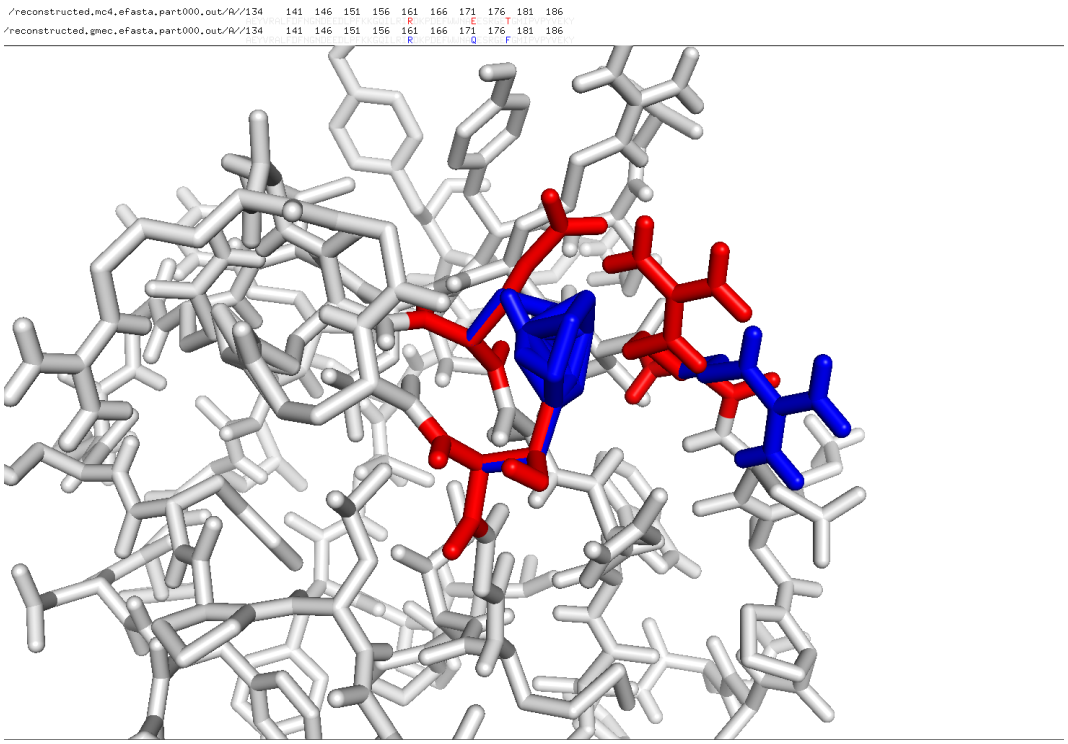

FIGURE 11 – test : 1CKA 5, GMEC vs MC

3.4 Résultats Superfamily

Protein	Match/seq size	Superfamily Evalue	superfamily success	Family Evalue	family success
1A81	no				
1ABO	51/58	4.4e-4	100%	2.8e-3	100%
1BM2	78/98	4.2e-5	100%	2.6e-3	100%
1CKA	40/57	1.1e-5	100%	3.4e-3.	100%
1G9O	79/91	7.0e-7	100%	2.5e-3	100%
1M61	97/109	7.2e-7	100%	2.6e-4	100%
1O4C	95/104	2.1e-4	100%	4.5e-3	100%
1R6J	74/82	9.8e-6	100%	4.6e-3	100%
2BYG	59/97	1.4e-5	100%	7.1e-3	100%

Protein	GMEC	H	MC	RE
1CKA 3	-304.6618	0	0	
1CKA 4	-302.4894	0	0	
1CKA 5	-299.2329	-0.2859	-3.2525	0
1G9O 3	-477.2503	-0.1366	0	
1G9O 4	-470.6458	0	0	
1G9O 5	-464.8659	0	-3.9599	0
1M61 1	-550.0699	0	-0.0776	
1M61 2	-538.6026	-3.5105	-4.5062	0.3215
1M61 5	-553.6559	0	-0.0432	

Protein	seq-rot nb gmec+1	H rank	MC rank	seq nb gmec+1	H mut nb	MC mut nb
1CKA 3	67669	1	1	227	0	0
1CKA 4	4649	1	1	498	0	0
1CKA 5	1388	78	?	77	0	2
1G9O 3	354559	23	1	63	1	0
1G9O 4	22639	1	1	381	0	0
1G9O 5	8658395	1	?	11	0	3
1M61 1	11199153	?	?	21	3	7
1M61 2	11199153	1	1	88	0	0
1M61 5	16417604	1	1	83	0	0

3.5 Résultats Heuristic (protocoles longs)

Proteins	GMEC	H	H+	H++
1ABO 1	-309.1670	-0.0675	-0.0675	0
1CKA 5	-299.2329	-0.2859	-0.0640	0
1G9O 3	-477.2503	-0.1366	0	0
1M61 2	-538.6026	-3.5105	-2.1673	-0.0188

TABLE 16 – Résultats pour 3 fois (resp 9 fois) plus de cycles heuristiques protocole H+ (resp H++)

3.6 densité en séquences

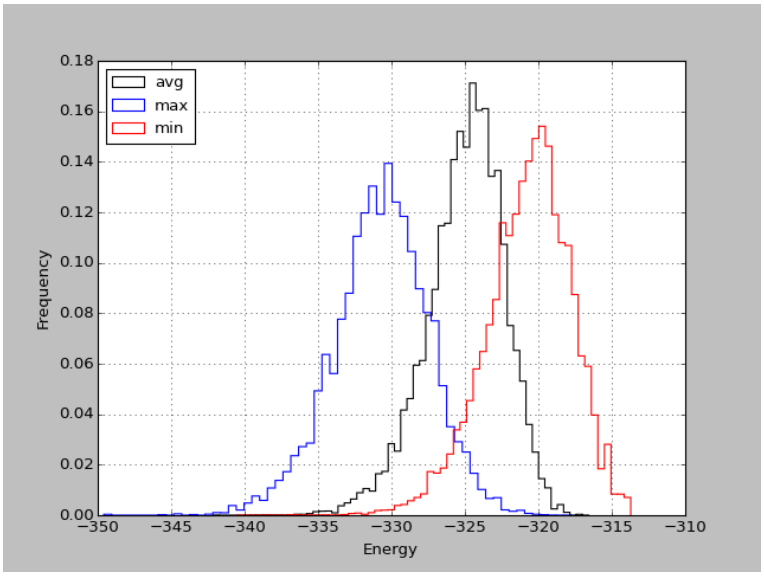

FIGURE 12 – .

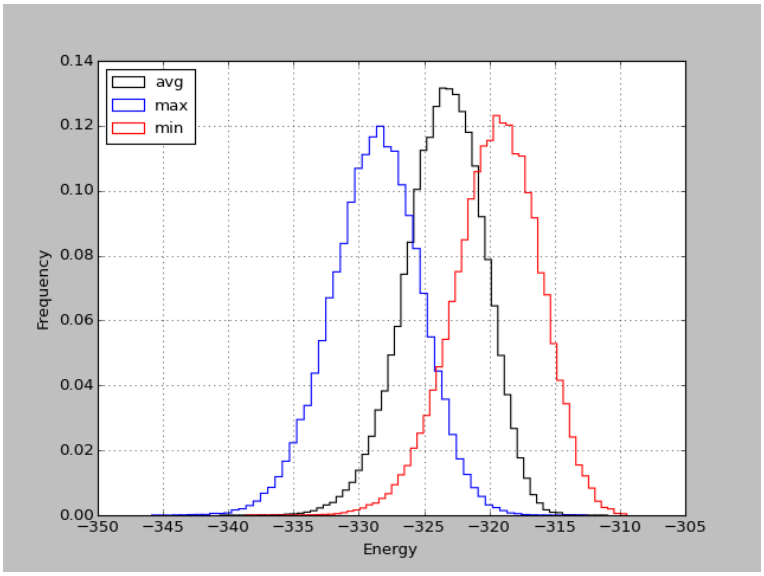

FIGURE 13 – .