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1 Les algorithmes

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

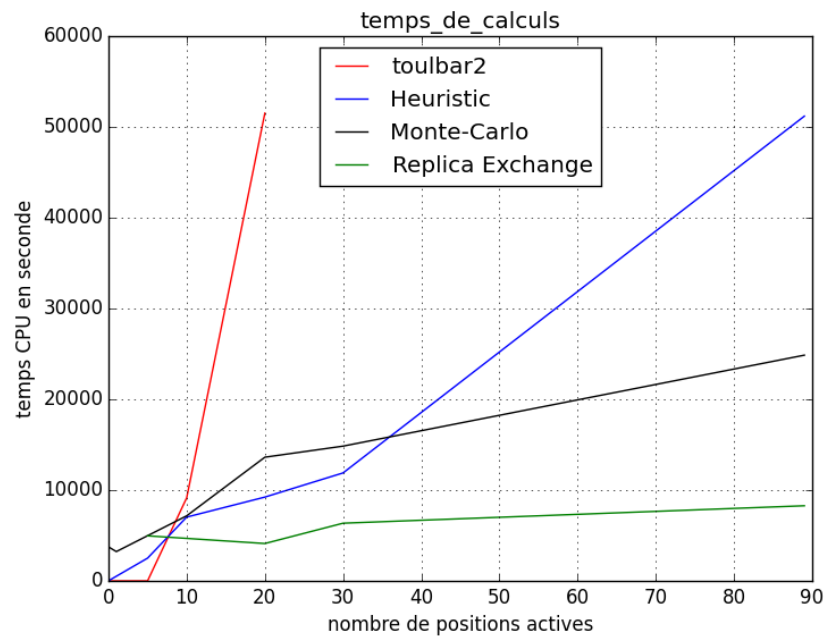


FIGURE 1 – Temps d’occupation du processeur selon le nombre de positions actives.

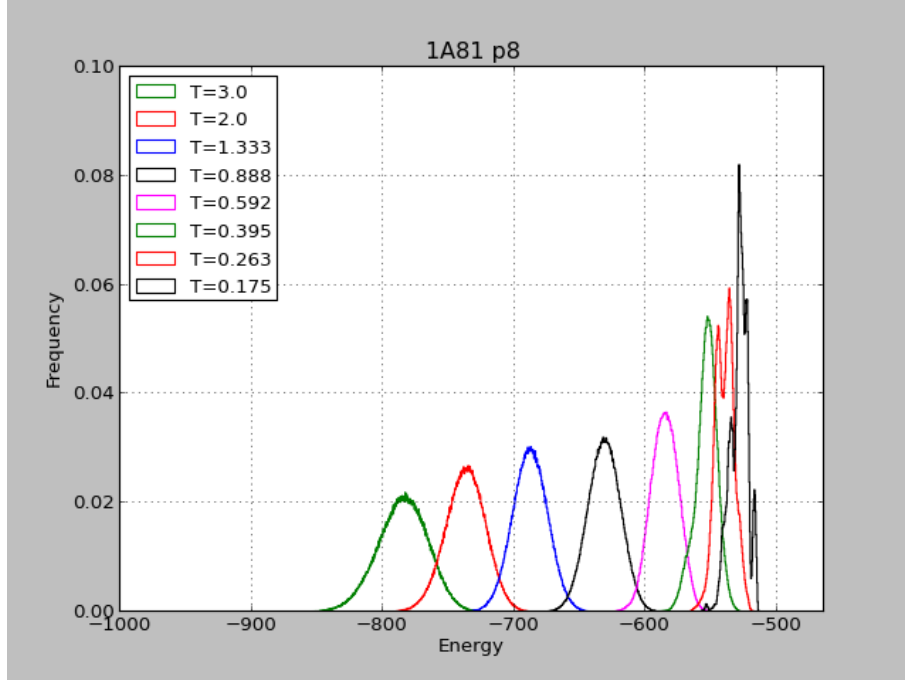


FIGURE 2 – Distribution des énergies selon la température (protocole RE3).

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

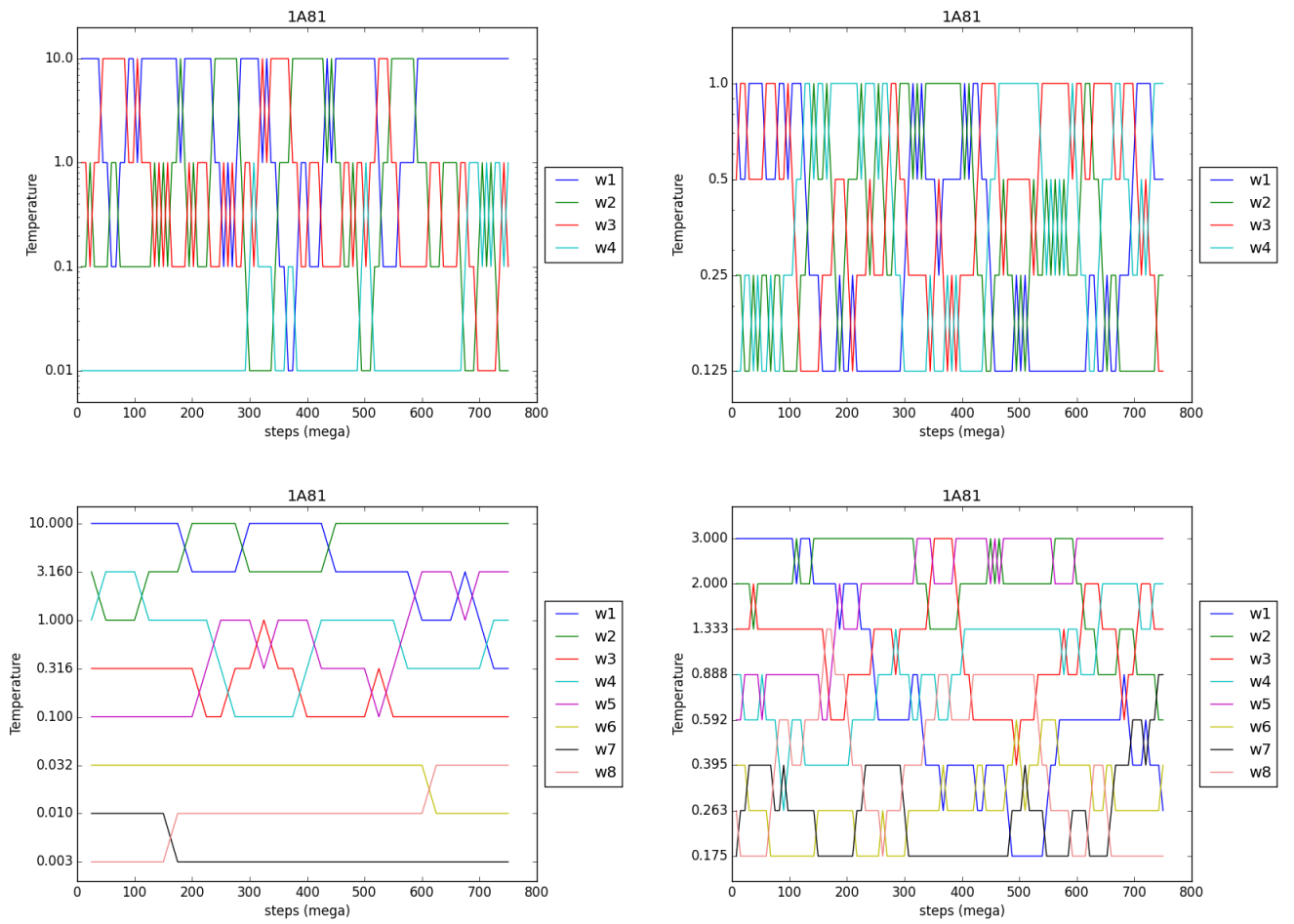


FIGURE 3 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

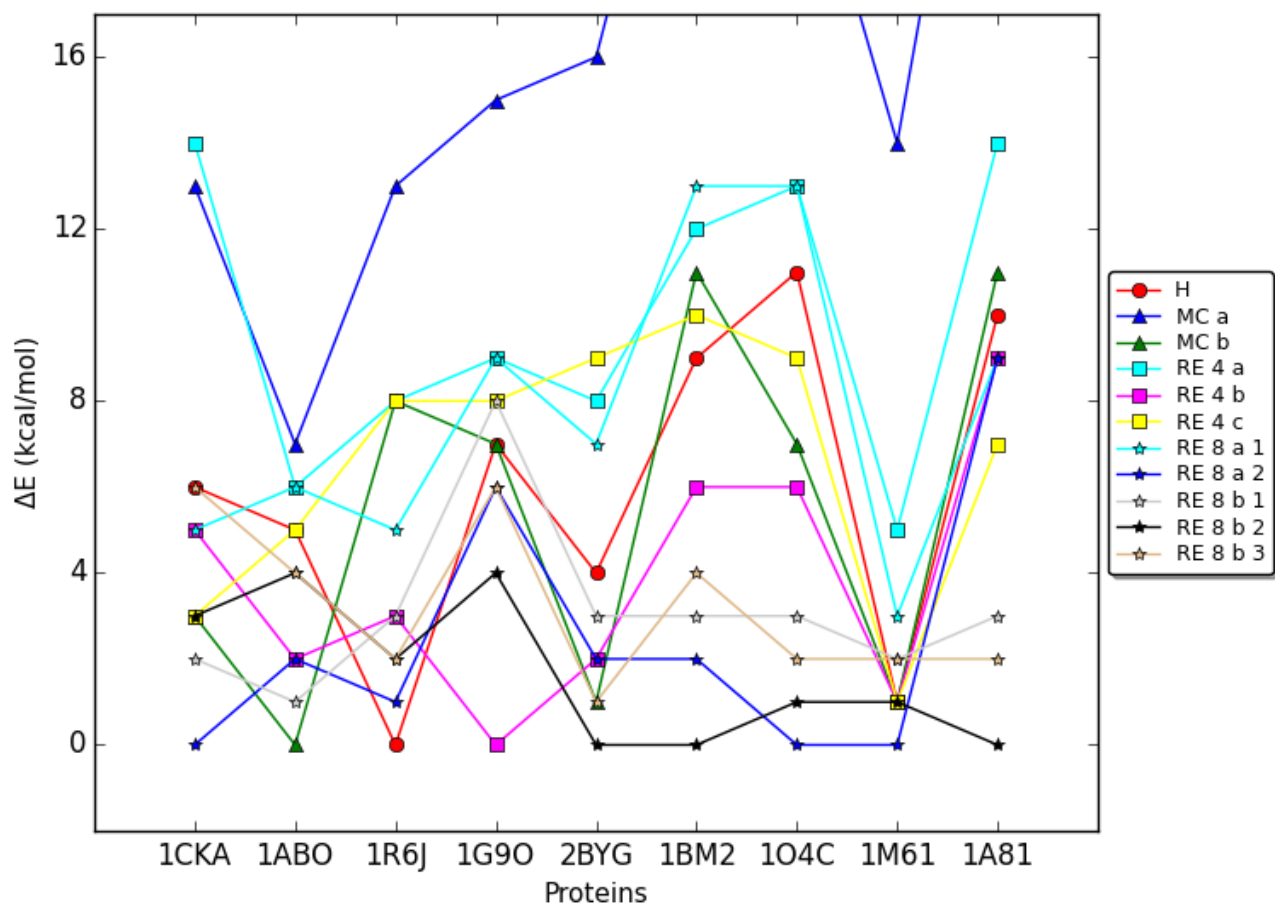


FIGURE 4 – Tous les protocoles.

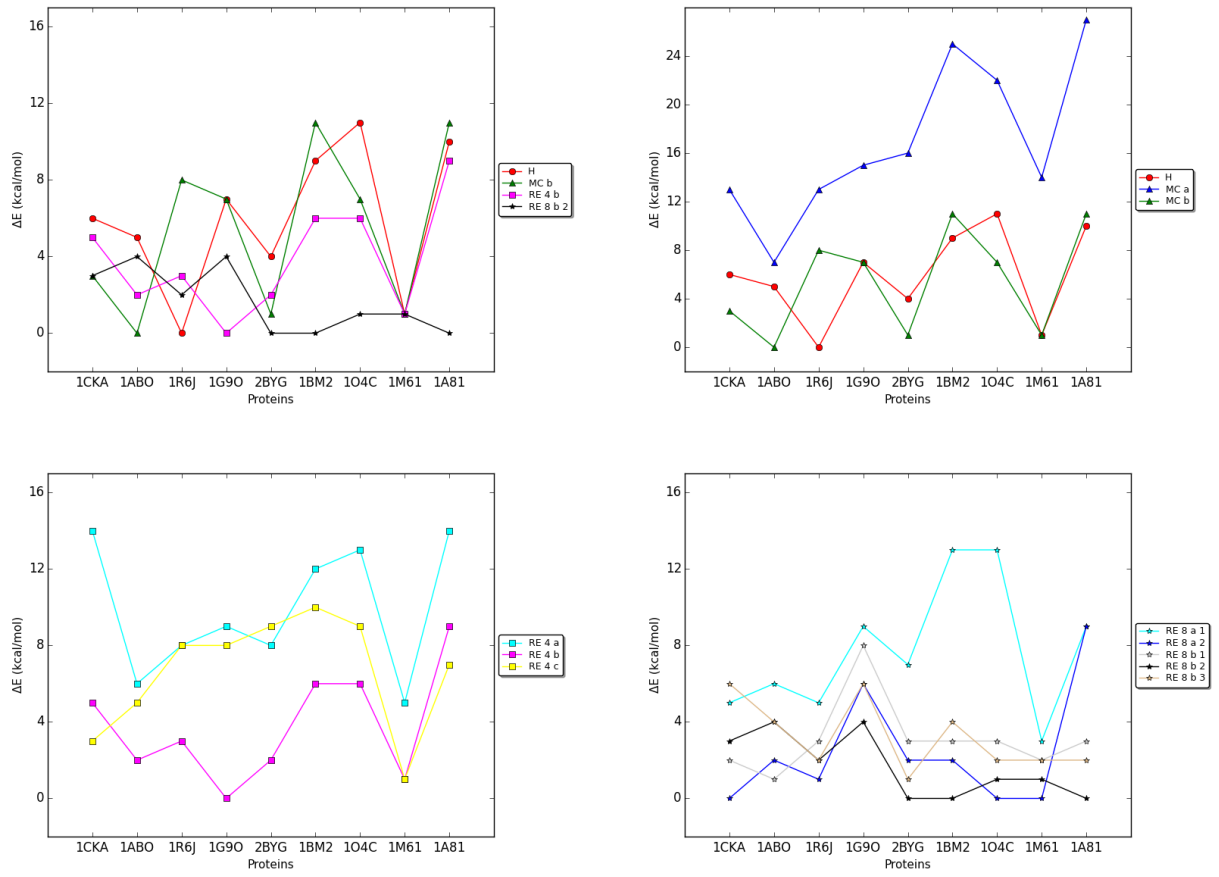


FIGURE 5 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

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 voisinage 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 | -590.16561 | -0.0807 |
| 51 | -591.1249 | -0.2986 |
| 52 | -589.7127 | -0.2734 |
| 53 | -590.7334 | -0.2019 |

| 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 | |
| 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 | 0.3215 |
| 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 | |
| 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 | -2.3986 |
| 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 | 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 | 0.3215 | -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 | | 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 | no |
| 1M61 2 | -538.6026 | -3.5105 | -4.5062 | | -528.7653 | 0 | 0 | no |
| 1M61 3 | -552.2673 | 0 | 0 | | -530.0684 | 0 | 0 | no |
| 1M61 4 | -550.0553 | 0 | 0 | | -534.5248 | 0 | 0 | no |
| 1M61 5 | -553.6559 | 0 | -0.0432 | | -548.0096 | 0 | -0.2521 | no |
| 1O4C 1 | -587.4665 | 0 | -0.1121 | -0.3986 | 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 | | -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 | 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 15 – Résultats 30 positions actives

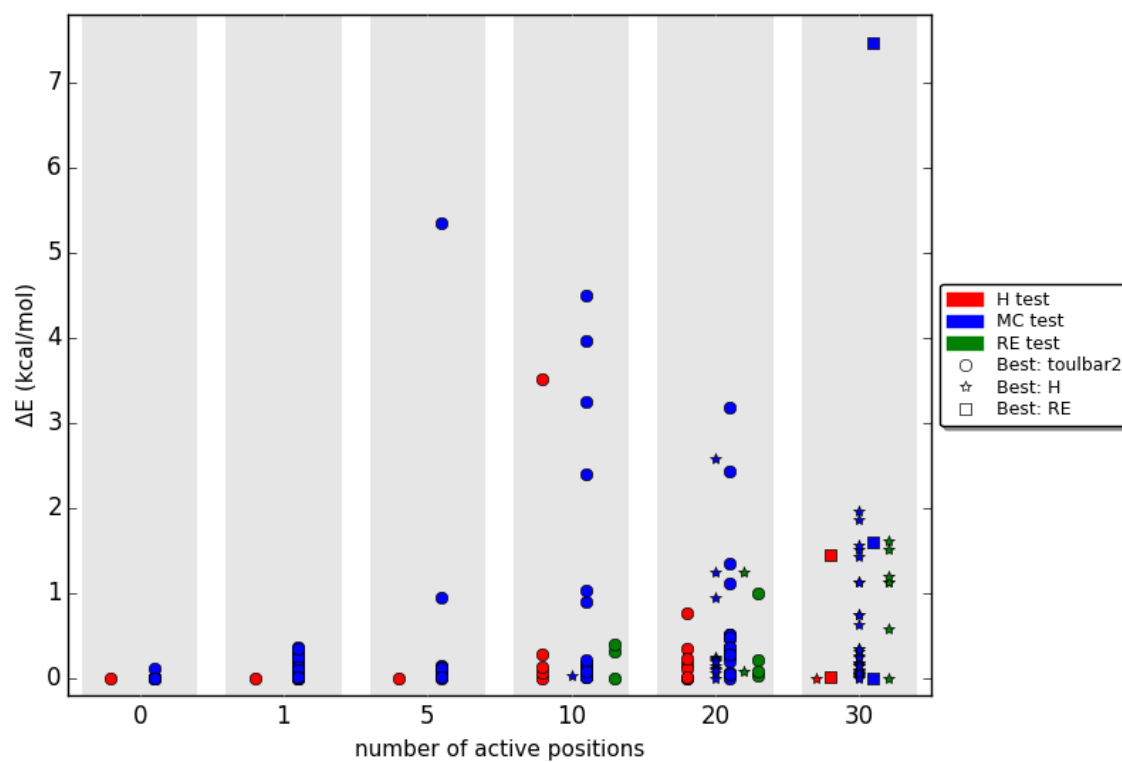


FIGURE 6 – Résultat d'ensemble des tests

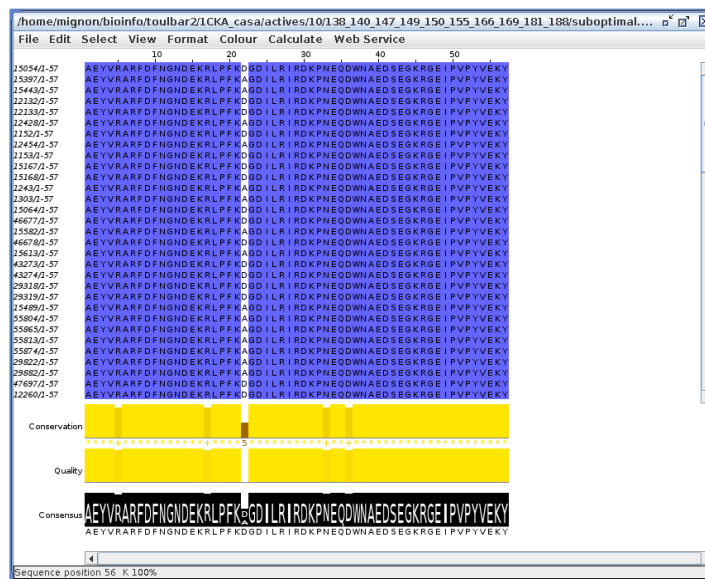


FIGURE 7 – .

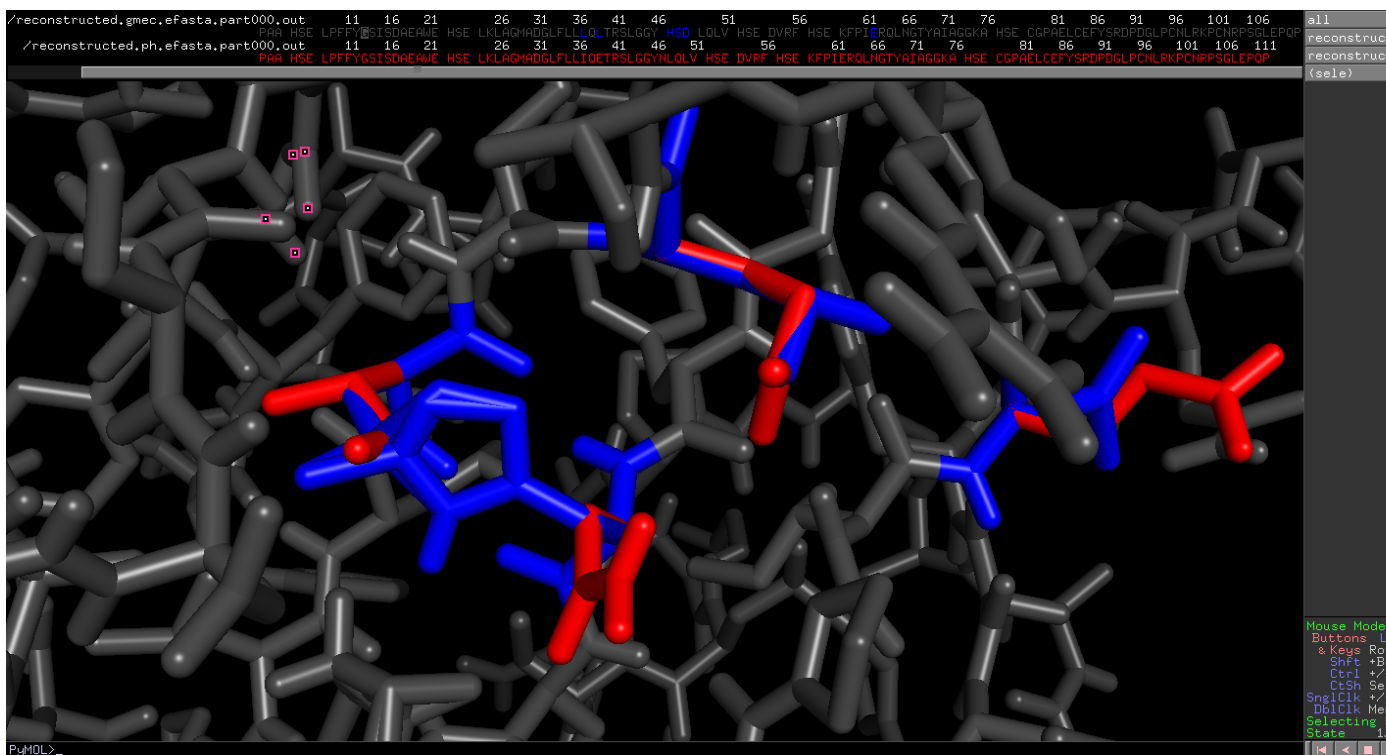


FIGURE 8 – .

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 | 0 |
| 1CKA 4 | -302.4894 | 0 | 0 | |
| 1CKA 5 | -299.2329 | -0.2859 | -3.2525 | |
| 1G9O 3 | -477.2503 | -0.1366 | 0 | |
| 1G9O 4 | -470.6458 | 0 | 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 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 | 0 |
| 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

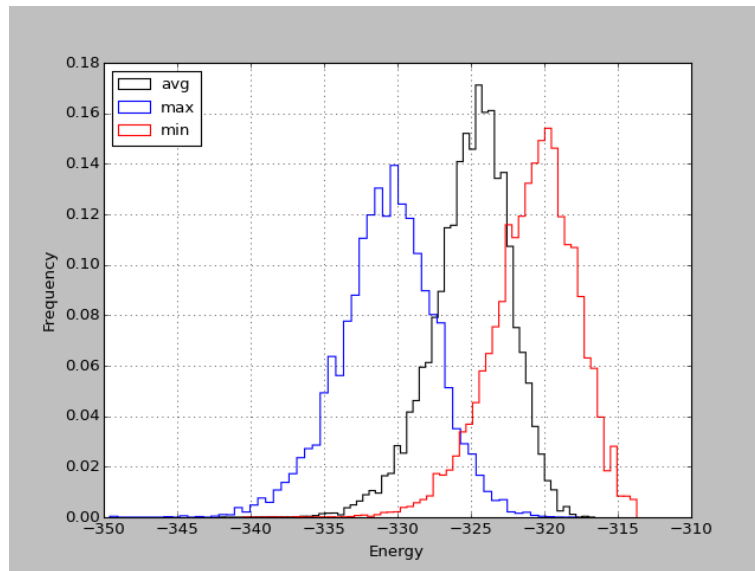


FIGURE 9 – .

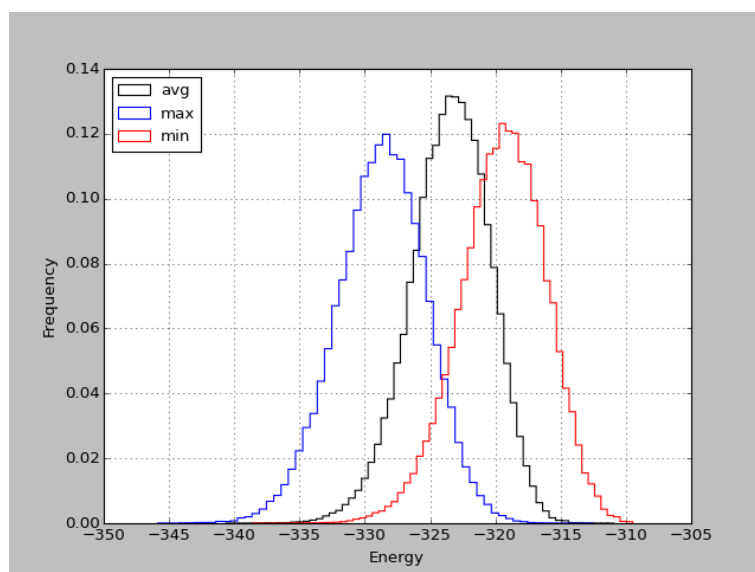


FIGURE 10 – .