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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

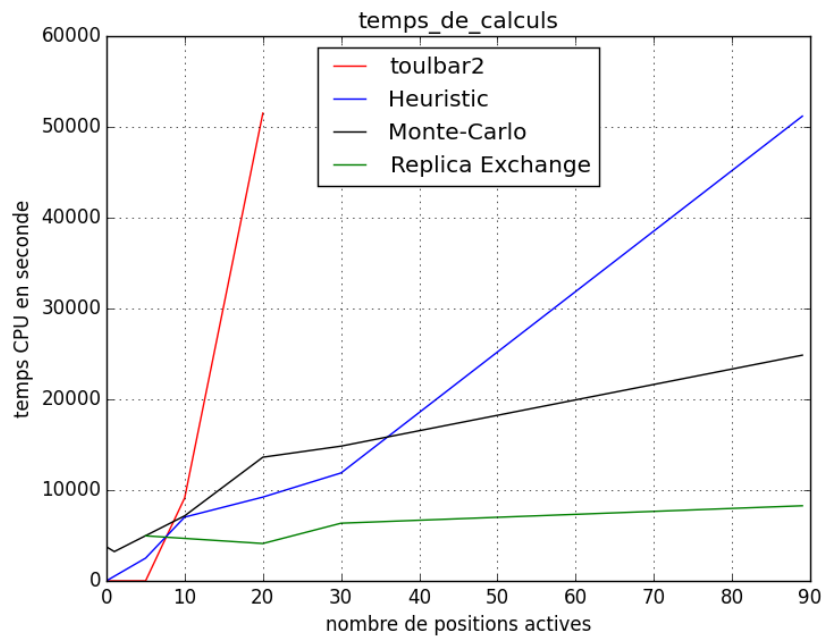


FIGURE 1 – Temps d’occupation du processeur selon le nombre de positions actives.

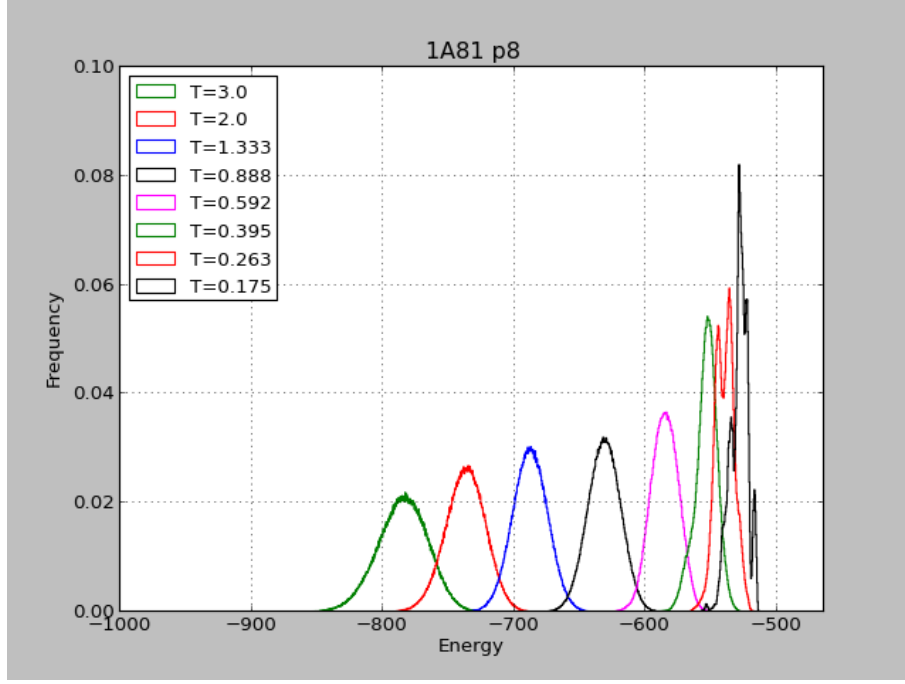


FIGURE 2 – Distribution des énergies selon la température (protocole RE3).

## 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

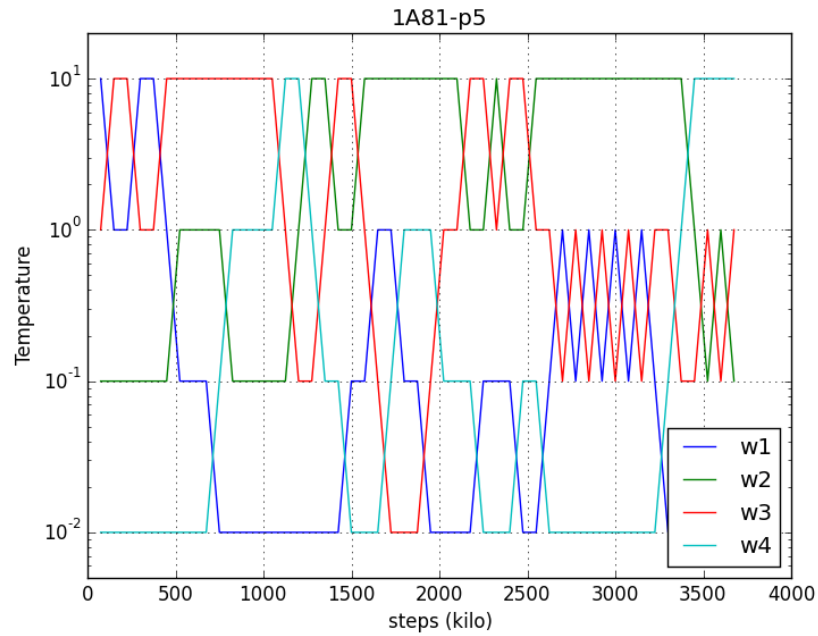


FIGURE 3 – Variation de la température au court de la trajectoire de chaque marcheur (protocole RE1).

### 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

| 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     |
|----------|-----------|---------|---------|
| 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 |
| 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 |
| 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       |
|----------|-----------|-----------|-----------|
| 1A81 1   | -566.9106 | 0         | -0.3275   |
| 1A81 2   | -564.6618 | -0.1705   | -2.4355   |
| 1A81 3   | -572.9780 | 0         | -0.4640   |
| 1A81 4   | -572.9780 | -0.3568   | -0.5088   |
| 1A81 5   | -572.9780 | -0.3568   | -0.5088   |
| 1ABO 1   | -299.6592 | -0.1205   | -1.1159   |
| 1ABO 2   | no        | -298.3854 | 0         |
| 1ABO 3   | no        | -298.3854 | no        |
| 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   |
| 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   | -295.8571 | 0         | 0         |
| 1CKA 2   | -295.8571 | 0         | 0         |
| 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        | -453.2474 | -0.2177   |
| 1G9O 3   | no        | -453.2474 | -0.2177   |
| 1G9O 4   | no        | -456.7331 | -0.1455   |
| 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   | -439.4335 | 0         | -0.0537   |
| 1R6J 5   | -438.0222 | 0         | -0.0735   |
| 2BYG 1   | -496.2991 | 0         | -3.1878   |
| 2BYG 2   | -494.8723 | 0         | -0.0524   |
| 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