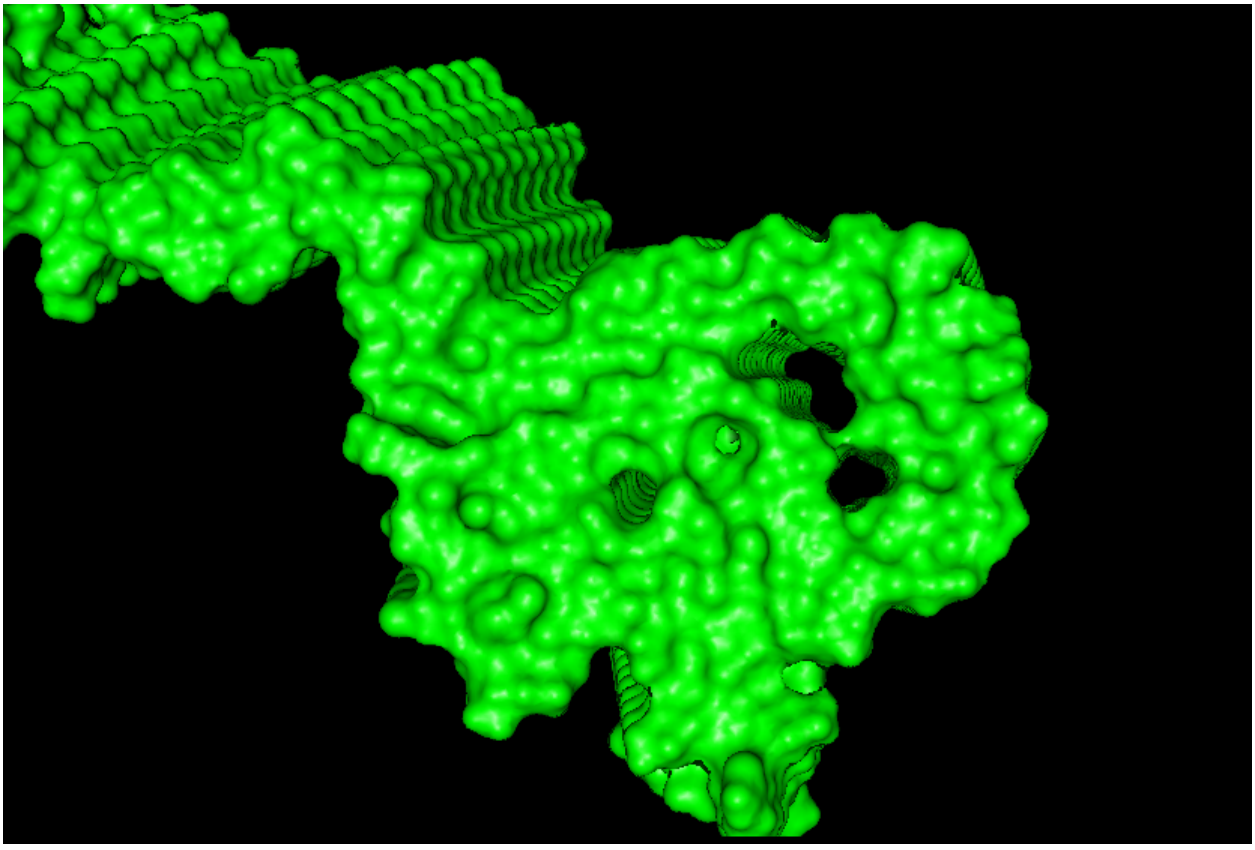
# 2N0A

Status Done

**Estructura:** 2N0A RCSB PDB - 2N0A: Atomic-resolution structure of alpha-synuclein fibrils. SOLID-STATE NMR.

**Análisis:** Posee dos túneles frecuentemente visitados por todos los ácidos grasos, incluidos los controles tioflavinaT y tioflavina TS2. Hay una tercera región hacia el extremo N-terminal.



**Conclusiones:** analizar los túneles en otras estructuras, así como la interacción con otros monómeros que puedan formar cavidades. Analizar distintas afinidades

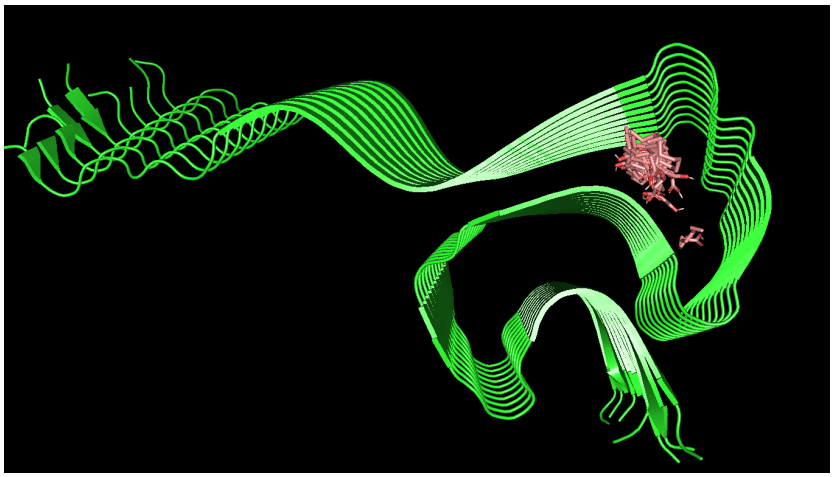
entre los ácidos grasos y según las regiones.

# SATURADOS

## Ácido Laurico (12:0) LA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | −5.2 | 0.000 | 0.000 |
| 2 | −4.6 | 9.453 | 11.233 |
| 3 | −4.4 | 12.659 | 14.205 |
| 4 | −4.4 | 9.618 | 10.877 |
| 5 | −4.4 | 21.473 | 23.394 |
| 6 | −4.3 | 20.190 | 22.407 |
| 7 | −4.3 | 12.531 | 15.799 |
| 8 | −4.3 | 15.678 | 18.088 |
| 9 | −4.3 | 10.675 | 11.700 |
| 10 | −4.3 | 8.991 | 11.848 |
| 11 | −4.1 | 20.770 | 24.256 |
| 12 | −4.1 | 10.796 | 12.982 |
| 13 | −4.1 | 19.913 | 23.730 |
| 14 | −4.1 | 11.347 | 13.609 |
| 15 | −4.1 | 8.771 | 11.845 |
| 16 | −4.0 | 23.830 | 26.079 |
| 17 | −4.0 | 11.338 | 13.352 |
| 18 | −4.0 | 14.293 | 17.958 |
| 19 | −4.0 | 14.986 | 17.149 |
| 20 | −3.9 | 10.207 | 11.198 |

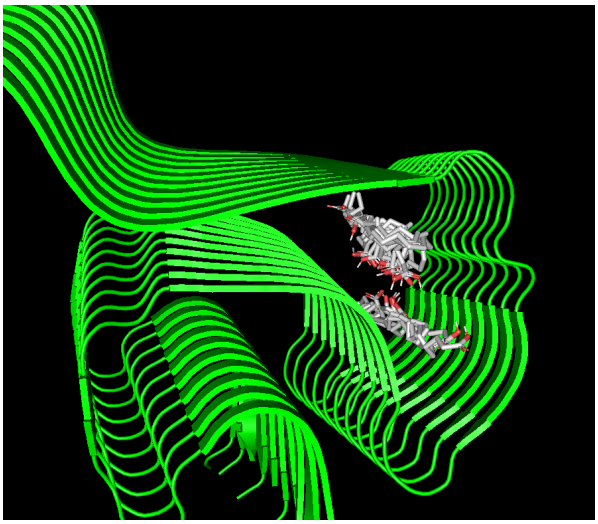
Writing output ... done.



## Ácido Mirístico (14:0) MA}

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.7 | 0.000 | 0.000 |
| 2 | -5.6 | 7.174 | 14.134 |
| 3 | -5.2 | 11.351 | 17.561 |
| 4 | -5.1 | 11.821 | 17.094 |
| 5 | -5.1 | 2.895 | 5.353 |
| 6 | -5.0 | 9.544 | 11.371 |
| 7 | -4.8 | 3.798 | 7.268 |
| 8 | -4.8 | 14.204 | 17.444 |
| 9 | -4.7 | 10.005 | 11.932 |
| 10 | -4.7 | 14.407 | 16.401 |
| 11 | -4.7 | 9.886 | 12.135 |
| 12 | -4.6 | 17.252 | 20.943 |
| 13 | -4.6 | 11.277 | 14.054 |
| 14 | -4.6 | 10.279 | 15.214 |
| 15 | -4.6 | 9.016 | 10.011 |
| 16 | -4.5 | 10.609 | 12.984 |
| 17 | -4.5 | 11.294 | 16.287 |
| 18 | -4.5 | 8.339 | 9.688 |
| 19 | -4.4 | 8.996 | 12.364 |
| 20 | -4.3 | 13.324 | 15.686 |

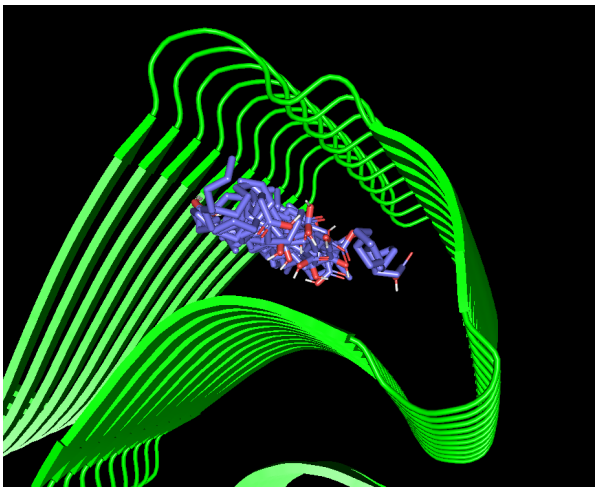
Writing output ... done.



# Ácido Palmítico (16:0) PA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.6 | 0.000 | 0.000 |
| 2 | -4.8 | 9.717 | 12.290 |
| 3 | -4.8 | 9.260 | 10.391 |
| 4 | -4.7 | 9.361 | 10.522 |
| 5 | -4.7 | 10.544 | 13.559 |
| 6 | -4.7 | 8.091 | 8.975 |
| 7 | -4.7 | 18.401 | 20.883 |
| 8 | -4.7 | 12.074 | 14.550 |
| 9 | -4.6 | 20.955 | 24.008 |
| 10 | -4.6 | 14.964 | 20.983 |
| 11 | -4.5 | 9.966 | 11.472 |
| 12 | -4.5 | 22.006 | 26.256 |
| 13 | -4.5 | 14.493 | 17.151 |
| 14 | -4.5 | 18.107 | 24.392 |
| 15 | -4.4 | 10.156 | 13.323 |
| 16 | -4.4 | 14.305 | 20.615 |
| 17 | -4.4 | 15.734 | 21.198 |
| 18 | -4.4 | 8.680 | 13.708 |
| 19 | -4.3 | 10.890 | 13.450 |
| 20 | -4.3 | 10.291 | 12.113 |

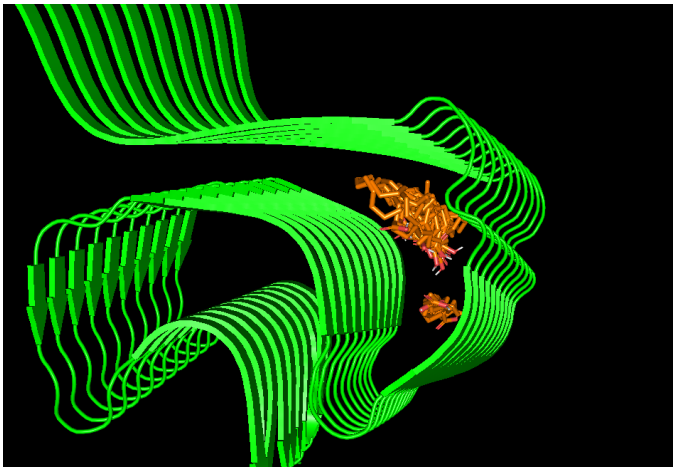
Writing output ... done.



## Ácido Esteáristico (18:0) SA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.7 | 0.000 | 0.000 |
| 2 | -5.7 | 9.443 | 13.754 |
| 3 | -5.6 | 1.168 | 2.111 |
| 4 | -5.5 | 10.228 | 14.144 |
| 5 | -5.3 | 9.558 | 10.856 |
| 6 | -5.3 | 10.221 | 13.347 |
| 7 | -5.3 | 9.494 | 10.512 |
| 8 | -5.2 | 9.524 | 14.394 |
| 9 | -5.2 | 11.025 | 16.658 |
| 10 | -5.2 | 10.501 | 13.230 |
| 11 | -5.2 | 6.117 | 11.953 |
| 12 | -5.1 | 9.270 | 10.256 |
| 13 | -5.1 | 9.967 | 11.220 |
| 14 | -5.1 | 9.036 | 11.633 |
| 15 | -5.1 | 17.087 | 21.099 |
| 16 | -5.1 | 9.700 | 13.360 |
| 17 | -5.0 | 9.642 | 12.798 |
| 18 | -4.9 | 10.008 | 12.378 |
| 19 | -4.9 | 10.854 | 14.165 |
| 20 | -4.9 | 13.520 | 20.501 |

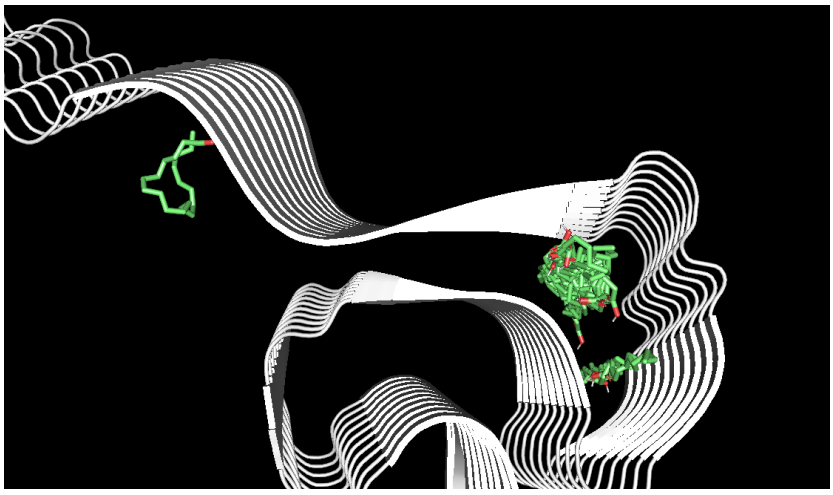
Writing output ... done.



## Ácido Araquídico (20:0) AqA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.5 | 0.000 | 0.000 |
| 2 | -5.3 | 11.202 | 23.020 |
| 3 | -5.3 | 9.971 | 13.305 |
| 4 | -5.3 | 9.466 | 10.465 |
| 5 | -5.3 | 10.519 | 16.794 |
| 6 | -5.3 | 9.700 | 11.303 |
| 7 | -5.2 | 12.311 | 15.000 |
| 8 | -5.2 | 10.017 | 14.639 |
| 9 | -5.1 | 16.268 | 20.864 |
| 10 | -5.1 | 22.979 | 27.478 |
| 11 | -5.0 | 18.634 | 22.681 |
| 12 | -5.0 | 43.272 | 44.573 |
| 13 | -5.0 | 15.567 | 19.254 |
| 14 | -5.0 | 11.043 | 15.928 |
| 15 | -5.0 | 18.956 | 25.952 |
| 16 | -4.9 | 23.589 | 26.671 |
| 17 | -4.9 | 10.522 | 15.669 |
| 18 | -4.9 | 9.425 | 12.481 |
| 19 | -4.9 | 19.640 | 25.194 |
| 20 | -4.8 | 22.310 | 27.533 |

Writing output ... done.



el 12 es el que aparece en la izquierda

# MUFAs:

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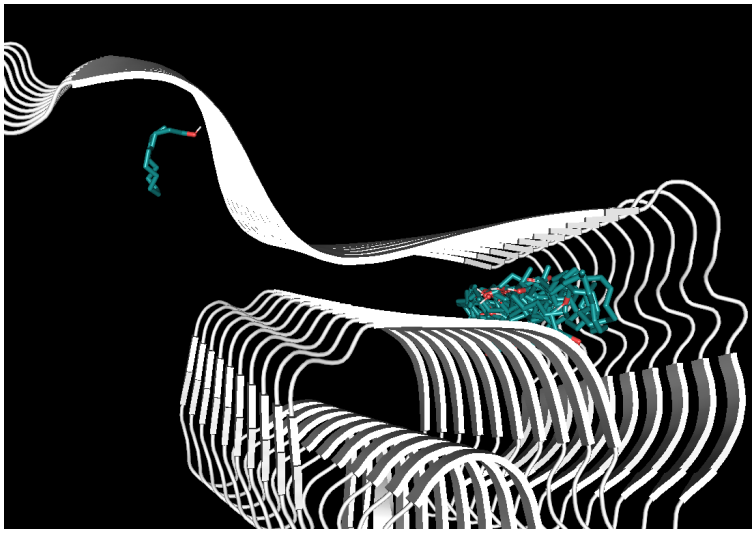
## Ácido Palmitoléico (16:1, n-7) PoA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -4.6 | 0.000 | 0.000 |
| 2 | -4.5 | 4.384 | 7.225 |
| 3 | -4.5 | 16.156 | 19.057 |
| 4 | -4.3 | 4.672 | 8.526 |
| 5 | -4.3 | 7.514 | 10.550 |
| 6 | -4.2 | 2.842 | 5.499 |
| 7 | -4.1 | 4.920 | 8.404 |
| 8 | -4.1 | 7.650 | 10.262 |
| 9 | -4.1 | 12.244 | 15.752 |
| 10 | -4.0 | 8.472 | 12.091 |
| 11 | -4.0 | 5.702 | 9.121 |
| 12 | -4.0 | 13.836 | 17.477 |
| 13 | -4.0 | 14.307 | 17.614 |
| 14 | -4.0 | 39.333 | 40.917 |
| 15 | -3.9 | 12.969 | 16.264 |
| 16 | -3.9 | 8.289 | 11.651 |
| 17 | -3.9 | 12.692 | 15.757 |
| 18 | -3.8 | 5.330 | 7.789 |
| 19 | -3.8 | 3.832 | 7.485 |
| 20 | -3.8 | 13.064 | 16.717 |

Writing output ... done.

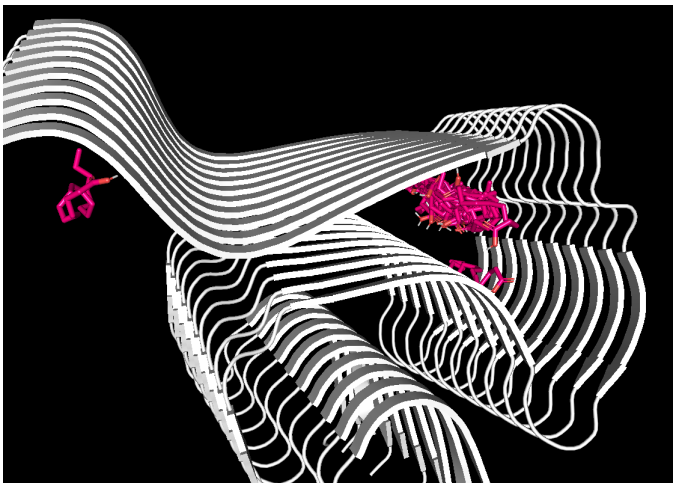


a la izquierda n°14

## Ácido Oléico (18:1,n-9) OA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.8 | 0.000 | 0.000 |
| 2 | -5.7 | 16.520 | 18.894 |
| 3 | -5.6 | 9.639 | 11.240 |
| 4 | -5.5 | 10.020 | 13.816 |
| 5 | -5.4 | 9.527 | 12.503 |
| 6 | -5.4 | 10.745 | 14.427 |
| 7 | -5.4 | 10.087 | 16.158 |
| 8 | -5.3 | 9.615 | 13.956 |
| 9 | -5.3 | 46.808 | 49.499 |
| 10 | -5.3 | 8.518 | 9.088 |
| 11 | -5.2 | 9.511 | 11.337 |
| 12 | -5.2 | 10.459 | 13.575 |
| 13 | -5.2 | 9.311 | 10.502 |
| 14 | -5.2 | 11.634 | 16.238 |
| 15 | -5.2 | 9.674 | 11.355 |
| 16 | -5.1 | 10.581 | 14.326 |
| 17 | -5.1 | 15.016 | 20.800 |
| 18 | -5.1 | 12.690 | 19.828 |
| 19 | -5.1 | 11.868 | 18.736 |
| 20 | -5.0 | 9.289 | 14.874 |

Writing output ... done.



n° 9 izquierda

# PUFAS:

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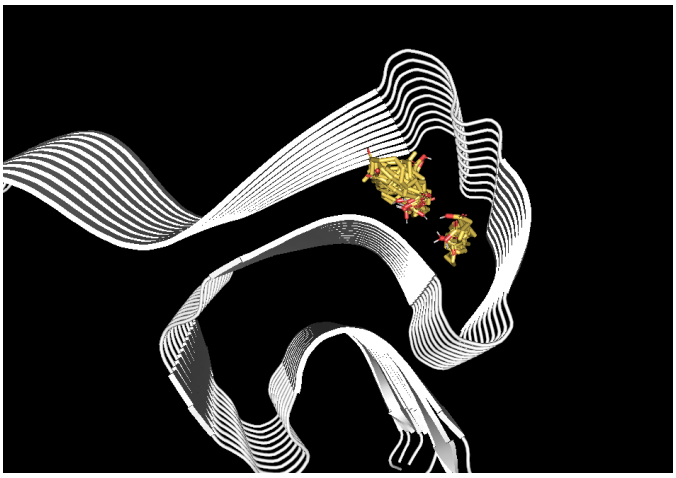
# Ácido Linoleico (18:2,n-6) LiA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -6.3 | 0.000 | 0.000 |
| 2 | -6.1 | 12.404 | 15.902 |
| 3 | -5.6 | 21.810 | 25.793 |
| 4 | -5.5 | 21.478 | 24.486 |
| 5 | -5.5 | 18.251 | 21.516 |
| 6 | -5.5 | 24.920 | 27.976 |
| 7 | -5.4 | 17.608 | 21.722 |
| 8 | -5.4 | 20.192 | 24.211 |
| 9 | -5.3 | 26.597 | 30.652 |
| 10 | -5.3 | 9.725 | 10.900 |
| 11 | -5.2 | 14.307 | 17.463 |
| 12 | -5.2 | 26.833 | 30.643 |
| 13 | -5.2 | 24.067 | 26.653 |
| 14 | -5.2 | 15.762 | 18.245 |
| 15 | -5.1 | 21.769 | 26.982 |
| 16 | -5.1 | 26.029 | 29.122 |
| 17 | -5.0 | 21.525 | 27.268 |
| 18 | -5.0 | 20.391 | 23.841 |
| 19 | -5.0 | 15.390 | 19.373 |
| 20 | -5.0 | 9.839 | 13.022 |

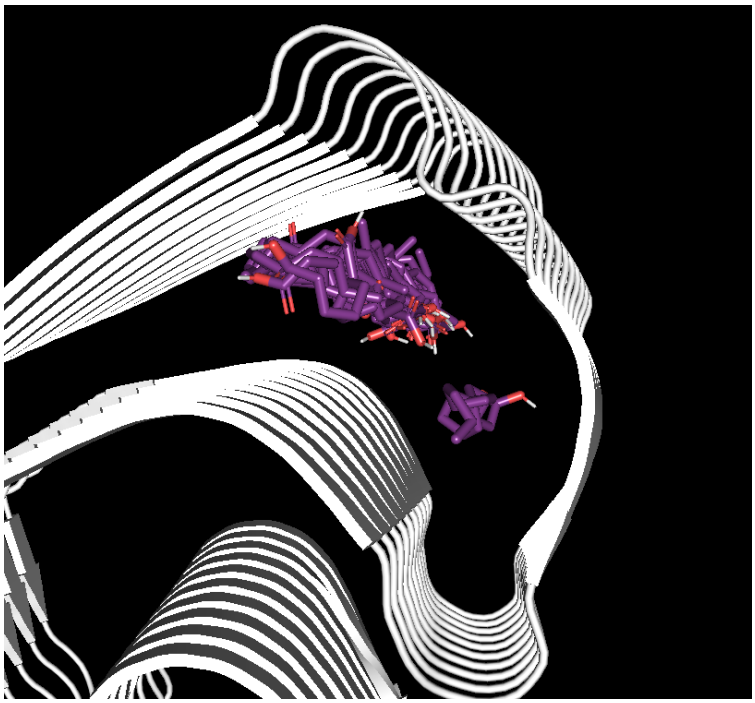
Writing output ... done.



# Ácido alfa-Linolénico (18:3,n-3) aLA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.9 | 0.000 | 0.000 |
| 2 | -5.6 | 8.589 | 10.651 |
| 3 | -5.6 | 10.339 | 15.221 |
| 4 | -5.5 | 8.809 | 10.175 |
| 5 | -5.4 | 8.735 | 10.038 |
| 6 | -5.4 | 8.740 | 12.073 |
| 7 | -5.4 | 10.221 | 15.856 |
| 8 | -5.3 | 15.958 | 21.371 |
| 9 | -5.2 | 17.285 | 21.526 |
| 10 | -5.2 | 8.763 | 11.599 |
| 11 | -5.2 | 10.283 | 14.701 |
| 12 | -5.1 | 11.231 | 14.988 |
| 13 | -5.1 | 14.166 | 20.131 |
| 14 | -5.1 | 17.853 | 23.178 |
| 15 | -5.0 | 12.387 | 15.641 |
| 16 | -5.0 | 19.088 | 22.003 |
| 17 | -5.0 | 9.933 | 14.113 |
| 18 | -5.0 | 13.520 | 18.368 |
| 19 | -4.9 | 7.808 | 9.047 |
| 20 | -4.9 | 11.266 | 13.781 |

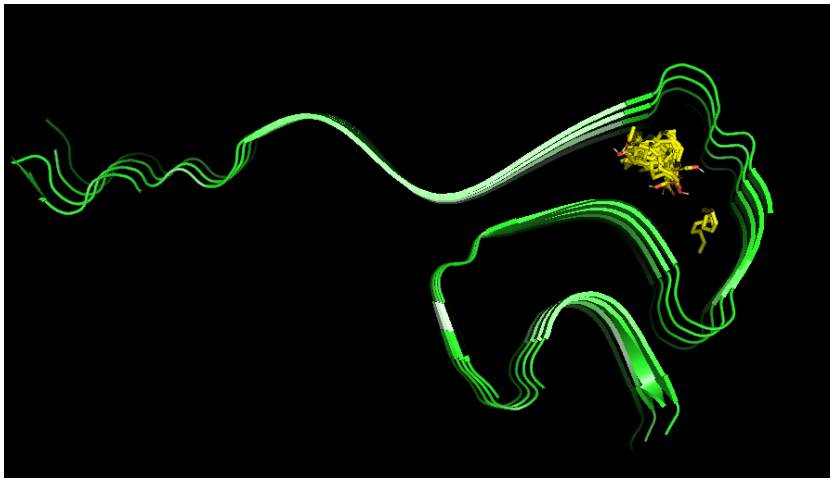
Writing output ... done.



# Ácido Araquidónico (20:4,n-6) ARA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.5 | 0.000 | 0.000 |
| 2 | -4.9 | 2.418 | 4.742 |
| 3 | -4.8 | 3.118 | 6.300 |
| 4 | -4.7 | 6.724 | 10.337 |
| 5 | -4.6 | 4.012 | 5.527 |
| 6 | -4.6 | 6.260 | 9.994 |
| 7 | -4.6 | 9.564 | 13.950 |
| 8 | -4.6 | 1.769 | 5.068 |
| 9 | -4.6 | 2.965 | 6.826 |
| 10 | -4.5 | 5.062 | 7.596 |
| 11 | -4.5 | 11.660 | 15.150 |
| 12 | -4.5 | 3.845 | 7.593 |
| 13 | -4.4 | 7.392 | 11.119 |
| 14 | -4.4 | 2.387 | 4.116 |
| 15 | -4.4 | 8.279 | 10.779 |
| 16 | -4.4 | 6.392 | 9.842 |
| 17 | -4.3 | 4.957 | 7.755 |
| 18 | -4.2 | 5.884 | 8.876 |
| 19 | -4.2 | 10.299 | 13.146 |
| 20 | -4.2 | 10.023 | 12.970 |

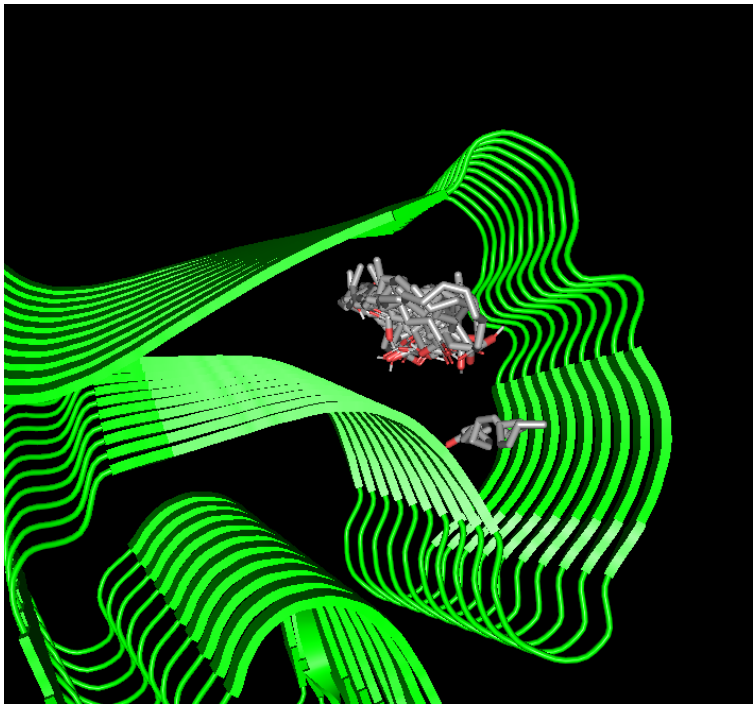
Writing output ... done.



# Ácido Eicosapentaenóico (20:5,n-3) EPA

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -6.9 | 0.000 | 0.000 |
| 2 | -6.2 | 11.010 | 15.952 |
| 3 | -6.1 | 9.524 | 11.308 |
| 4 | -6.1 | 13.367 | 20.198 |
| 5 | -6.0 | 10.872 | 14.348 |
| 6 | -6.0 | 9.795 | 10.757 |
| 7 | -5.9 | 13.282 | 18.260 |
| 8 | -5.9 | 14.665 | 19.590 |
| 9 | -5.8 | 9.914 | 12.290 |
| 10 | -5.8 | 9.649 | 11.445 |
| 11 | -5.8 | 10.263 | 12.973 |
| 12 | -5.8 | 13.755 | 16.739 |
| 13 | -5.7 | 10.242 | 14.992 |
| 14 | -5.7 | 16.520 | 20.541 |
| 15 | -5.7 | 10.734 | 14.701 |
| 16 | -5.6 | 12.637 | 18.191 |
| 17 | -5.6 | 11.559 | 15.455 |
| 18 | -5.6 | 9.681 | 12.055 |
| 19 | -5.6 | 11.776 | 16.990 |
| 20 | -5.5 | 9.430 | 12.748 |

Writing output ... done.



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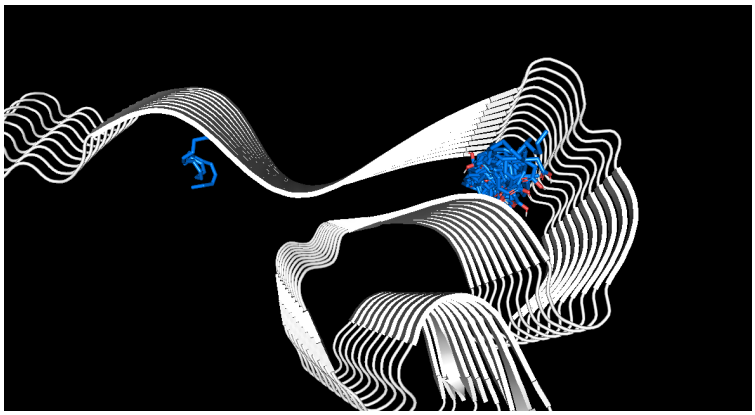
## Ácido Docosahexaenóico (22:6,n-3) DHA

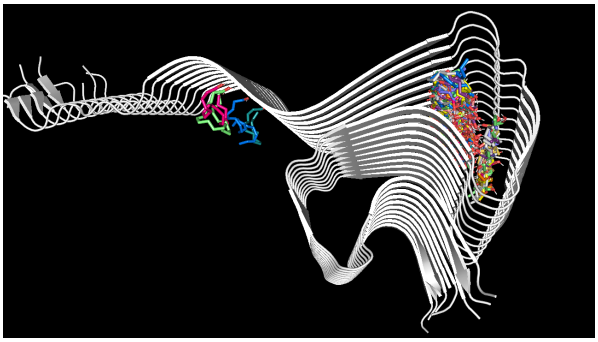
| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -5.8 | 0.000 | 0.000 |
| 2 | -5.5 | 3.582 | 8.096 |
| 3 | -5.4 | 4.621 | 8.804 |
| 4 | -5.4 | 7.594 | 13.625 |
| 5 | -5.3 | 10.445 | 14.281 |
| 6 | -5.3 | 2.535 | 6.457 |
| 7 | -5.2 | 9.850 | 15.917 |
| 8 | -5.1 | 7.964 | 12.026 |
| 9 | -5.1 | 10.078 | 14.787 |
| 10 | -5.1 | 1.903 | 4.670 |
| 11 | -5.1 | 12.266 | 17.919 |
| 12 | -5.1 | 3.048 | 5.221 |
| 13 | -5.1 | 1.623 | 2.975 |
| 14 | -5.0 | 7.819 | 13.854 |
| 15 | -5.0 | 6.214 | 9.811 |
| 16 | -5.0 | 7.989 | 12.455 |
| 17 | -5.0 | 6.974 | 13.346 |
| 18 | -4.9 | 36.319 | 38.768 |
| 19 | -4.8 | 2.388 | 4.886 |
| 20 | -4.7 | 9.764 | 15.717 |

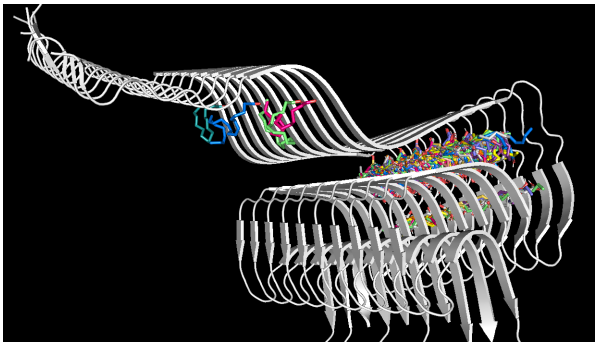
Writing output ... done.



n°18

## TODOS



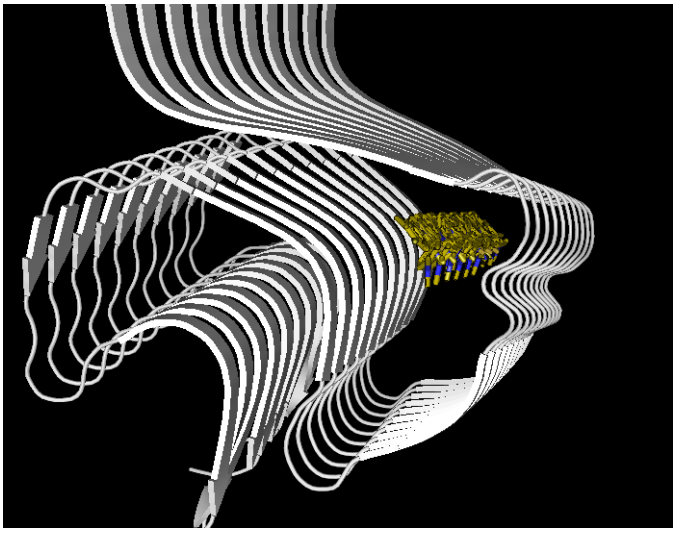


# Control

## Tioflavina T

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -6.9 | 0.000 | 0.000 |
| 2 | -6.9 | 3.017 | 5.106 |
| 3 | -6.9 | 15.016 | 19.759 |
| 4 | -6.9 | 6.396 | 9.930 |
| 5 | -6.9 | 2.890 | 4.896 |
| 6 | -6.9 | 10.431 | 14.858 |
| 7 | -6.8 | 11.218 | 16.982 |
| 8 | -6.8 | 2.705 | 7.379 |
| 9 | -6.8 | 2.296 | 7.847 |
| 10 | -6.8 | 7.173 | 12.797 |
| 11 | -6.8 | 15.777 | 21.552 |
| 12 | -6.8 | 3.164 | 8.151 |
| 13 | -6.8 | 4.148 | 9.590 |
| 14 | -6.8 | 3.844 | 9.099 |
| 15 | -6.8 | 3.285 | 8.669 |
| 16 | -6.8 | 16.302 | 22.338 |
| 17 | -6.8 | 1.571 | 2.528 |
| 18 | -6.8 | 12.389 | 17.064 |
| 19 | -6.8 | 16.991 | 21.944 |
| 20 | -6.7 | 8.033 | 12.138 |

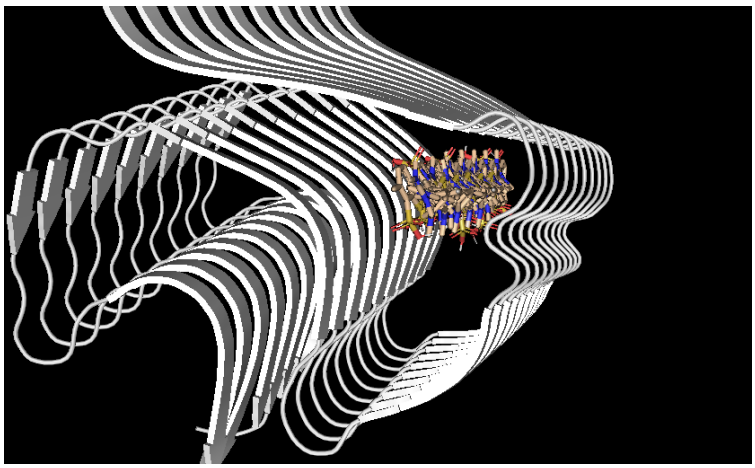
Writing output ... done.



## Tioflavina S2

| mode | affinity (kcal/mol) | dist from best mode rmsd l.b. | rmsd u.b. |
|---|---|---|---|
| 1 | -10.1 | 0.000 | 0.000 |
| 2 | -10.1 | 5.450 | 9.842 |
| 3 | -10.1 | 2.621 | 5.044 |
| 4 | -10.0 | 2.501 | 4.812 |
| 5 | -10.0 | 5.828 | 12.525 |
| 6 | -10.0 | 4.291 | 11.567 |
| 7 | -10.0 | 8.122 | 15.148 |
| 8 | -10.0 | 4.007 | 12.608 |
| 9 | -9.9 | 11.131 | 18.725 |
| 10 | -9.9 | 5.453 | 9.856 |
| 11 | -9.9 | 3.331 | 6.129 |
| 12 | -9.9 | 4.454 | 13.042 |
| 13 | -9.8 | 9.398 | 16.664 |
| 14 | -9.8 | 2.996 | 5.512 |
| 15 | -9.8 | 6.895 | 13.624 |
| 16 | -9.8 | 4.356 | 11.656 |
| 17 | -9.8 | 7.670 | 14.569 |
| 18 | -9.8 | 10.441 | 17.912 |
| 19 | -9.7 | 4.863 | 11.797 |
| 20 | -9.7 | 4.592 | 13.466 |

Writing output ... done.



# Archivos

prueba02.pse