Potential activity of Linezolid against SARS-CoV-2 using electronic and molecular docking study

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Figure S1: Column chart for conformational structures in relation to the value of binding energy for the results obtained in the studies of molecular docking for the (R)-Linezolid (a) and (S)-Linezolid (b) structures.
Figure S2: Interactions of the conformational structure of (S)-Linezolid from molecular docking, by Discovery Studio Visualizer 2019 software.
Figure S3: (R)-Linezolid LigPlot+.
**Table S1.** Cartesian Coordinates (in Å) of (R)-Linezolid obtained at [B3LYP/6-311++G(2d,p) + GD3BJ] level of theory.

| At. Simb. | X       | Y       | Z       |
|-----------|---------|---------|---------|
| C         | 0.000000| 0.000000| 0.000000|
| N         | 0.000000| 0.000000| 3.718632|
| O         | 0.709165| 0.000000| 5.860691|
| C         | -0.763907| 1.147294| -0.293555|
| N         | 1.632890| -2.699092| 4.131085|
| O         | 1.198588| 1.831748| 4.616942|
| C         | -1.267157| 1.902253| 0.784109|
| N         | -1.018522| 1.526753| -1.615647|
| O         | 3.475908| -1.353382| 3.680863|
| C         | -1.015653| 1.524412| 2.103428|
| O         | -1.386553| 2.065784| -4.350985|
| C         | -0.256611| 0.386275| 2.371748|
| C         | 0.251635| -0.375627| 1.319037|
| C         | -0.541809| -1.198193| 4.302870|
| C         | 0.225004| -1.325827| 5.602003|
| C         | 0.687686| 0.722403| 4.688488|
| C         | 1.413485| -2.272413| 5.505622|
| C         | 2.647822| -2.196575| 3.346115|
| C         | 2.664139| -2.826040| 1.978452|
| C         | 0.122462| 1.921840| -2.455835|
| C         | -0.370683| 2.762035| -3.629144|
| C         | -2.524204| 1.836060| -3.519013|
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| C | -2.153938  | 0.944665   | -2.339715  |
| F | 0.494466   | -0.738622  | -1.003636  |
| H | 1.000138   | -3.395192  | 3.746439   |
| H | 0.835310   | -1.248418  | 1.524156   |
| H | -1.860983  | 2.794297   | 0.584219   |
| H | -1.413635  | 2.119974   | 2.925404   |
| H | -0.440319  | -2.072139  | 3.659095   |
| H | -1.610992  | -1.095085  | 4.487744   |
| H | -0.418198  | -1.732335  | 6.381852   |
| H | 1.204732   | -3.153280  | 6.112047   |
| H | 2.306393   | -1.762250  | 5.867466   |
| H | 2.109710   | -2.196514  | 1.282211   |
| H | 3.693523   | -2.925408  | 1.635856   |
| H | 2.199766   | -3.810804  | 2.025861   |
| H | 0.618346   | 1.028086   | -2.835570  |
| H | 0.825786   | 2.505502   | -1.861779  |
| H | 0.466962   | 2.956630   | -4.298883  |
| H | -0.776503  | 3.701329   | -3.252840  |
| H | -2.798794  | 2.785197   | -3.109254  |
| H | -3.226690  | 1.284953   | -4.108878  |
| H | -2.455469  | 0.422621   | -1.431749  |
| H | -2.498930  | 0.263574   | -3.089009  |
**Table S2.** Cartesian Coordinates (in Å) of (S)-Linezolid obtained at [B3LYP/6-311++G(2d,p) + GD3BJ] level of theory.

| At. Simb. | X       | Y       | Z       |
|-----------|---------|---------|---------|
| C         | 0.000000| 0.000000| 0.000000|
| N         | 0.000000| 0.000000| 2.274239|
| O         | 1.410110| 0.000000| 0.297002|
| C         | -0.579031| -0.758163| 1.184318|
| N         | -0.263245| -2.660999| 7.355576|
| O         | 2.358109 | 0.498611| 2.446402|
| C         | 1.359919 | 0.197710| 1.740466|
| N         | 0.929585 | -0.944960| 2.069451|
| O         | -0.970673| -4.902651| 8.973270|
| C         | -0.066654| -0.681046| 3.574508|
| O         | 0.163195 | -3.181235| -2.124039|
| C         | -0.404605| -2.039980| 3.636750|
| C         | -0.467951| -2.689216| 4.878420|
| C         | -0.195838| -1.980305| 6.054105|
| C         | 0.140774 | -0.620794| 5.991772|
| C         | 0.206062 | 0.027606| 4.751433|
| C         | -1.661106| -2.959379| 7.685241|
| C         | -1.718274| -3.681695| 9.044607|
| C         | 0.400588 | -4.626091| 8.662909|
| C         | 0.489633 | -3.917846| 7.298643|
| C         | -0.322734| -0.658969| -1.354647|
| C         | 0.855098 | -2.283705| -2.671753|
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 1.621880 | -2.588382 | -3.971424 |
| F    | 0.404016  | 0.062134  | 7.126860   |
| H    | -0.419084 | 0.999741  | -0.113951  |
| H    | -0.358201 | -1.825458 | 1.198912   |
| H    | -1.668269 | -0.719531 | 1.197217   |
| H    | -0.617955 | -2.591607 | 2.721170   |
| H    | -0.729208 | -3.746293 | 4.927766   |
| H    | 0.469222  | 1.084221  | 4.702394   |
| H    | -2.090691 | -3.598017 | 6.913422   |
| H    | -2.229462 | -2.030946 | 7.740720   |
| H    | -2.755938 | -3.907195 | 9.290589   |
| H    | -1.292381 | -3.039417 | 9.815448   |
| H    | 0.957439  | -5.562178 | 8.621018   |
| H    | 0.825222  | -3.983670 | 9.434326   |
| H    | 1.533134  | -3.708005 | 7.063732   |
| H    | 0.068700  | -4.560663 | 6.525528   |
| H    | -0.935778 | 0.016793  | -1.950995  |
| H    | -0.867085 | -1.588349 | -1.187210  |
| H    | 2.293439  | -1.760537 | -4.198967  |
| H    | 2.202348  | -3.502363 | -3.845739  |
| H    | 0.913834  | -2.716654 | -4.790152  |
| H    | 1.696135  | -0.909811 | -1.428480  |