**Supplemental Files**

**Tackling the SARS-CoV-2 main protease using hybrid derivatives of 1,5-disubstituted tetrazole-1,2,3-triazoles: an *in silico* assay**

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**Cartesian cordinates**

Compound 1e

C -9.92730 15.56110 68.68180

N -9.31700 16.50170 67.77190

N -8.03190 16.58440 68.34200

N -7.91900 15.84870 69.36860

N -9.11540 15.18220 69.61510

H -9.19530 18.47870 65.87830

C -11.34190 15.02120 68.51650

H -11.36450 14.11180 69.15650

H -11.90900 12.48570 67.65700

N -12.37060 15.93240 69.06410

H -11.94630 19.56330 66.78010

H -10.77370 17.62050 65.80050

H -8.19540 19.04530 68.28820

H -9.14230 18.53020 69.72850

H -9.38400 20.96940 69.25120

H -10.95690 20.10240 69.17180

H -9.18450 20.96060 66.78340

C -9.22360 18.88170 68.67790

H -14.66440 10.94420 73.21240

C -9.96940 20.22190 68.67380

N -11.39340 7.06810 70.72130

C -10.17200 20.73500 67.24300

C -11.68690 14.56840 67.10130

C -11.74480 15.47220 66.02330

C -12.07060 15.03140 64.73800

C -12.36890 13.67020 64.50110

C -12.27690 12.76940 65.56800

C -11.95140 13.21030 66.85330

H -13.74680 8.71700 72.72940

H -12.07210 15.75540 63.93500

H -12.47140 11.71730 65.40160

H -10.99170 17.69780 68.25360

C -12.21580 16.24090 70.49510

H -13.30550 15.48150 68.92210

H -12.77200 17.16580 70.74520

H -11.14460 16.36630 70.76300

C -13.59050 14.17490 70.92520

C -12.79380 15.14360 71.34390

N -12.53720 14.93890 72.72140

N -13.17010 13.89300 73.06910

N -13.91230 13.30470 72.02320

H -13.95760 14.05220 69.91060

H -10.99430 20.07900 65.34510

C -13.40380 11.97840 71.77580

C -12.39920 11.81280 70.81300

C -11.87920 10.54370 70.54040

C -12.36110 9.42370 71.22890

C -13.36620 9.57700 72.19120

C -13.88760 10.84490 72.46510

H -12.01870 12.67160 70.27430

H -11.10200 10.43620 69.79320

C -11.82470 8.11800 70.94750

H -10.75960 21.67780 67.27160

C -9.97600 17.82910 67.81750

C -10.91490 19.70200 66.38740

C -10.17830 18.35620 66.38390

O -12.65770 13.15110 63.24300

H -11.52380 16.52150 66.16930

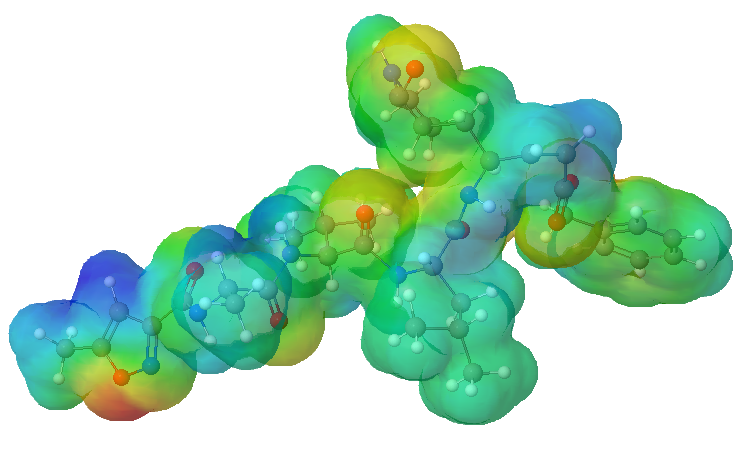
C -12.81040 11.74790 63.27020

H -12.68730 11.36250 62.23740

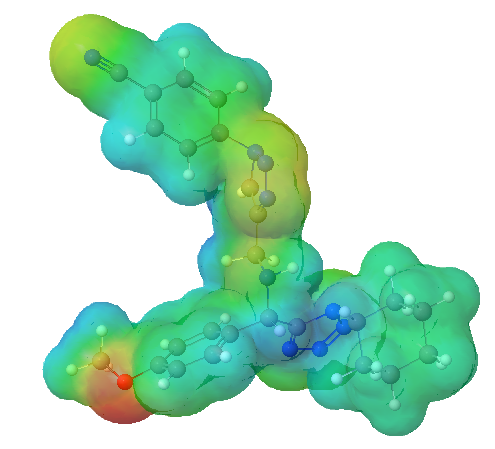
H -13.83420 11.47380 63.60240

H -12.03840 11.25070 63.90130

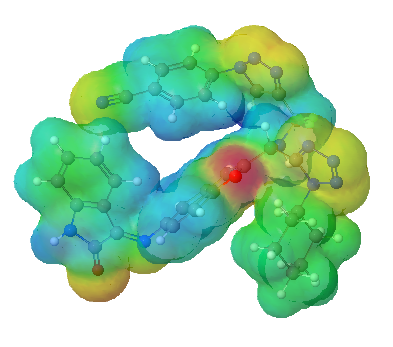
**Molecular electrostatic potential surfaces**



**Fig. S1**. Molecular electrostatic potential surface for the co-crystalized molecule (into the SARS-CoV-2-MPro).



**Fig. S2**. Molecular electrostatic potential surface for the 1e molecule.



**Fig. S3**. Molecular electrostatic potential surface for the P8 molecule.