

Supplemental data for the manuscript:

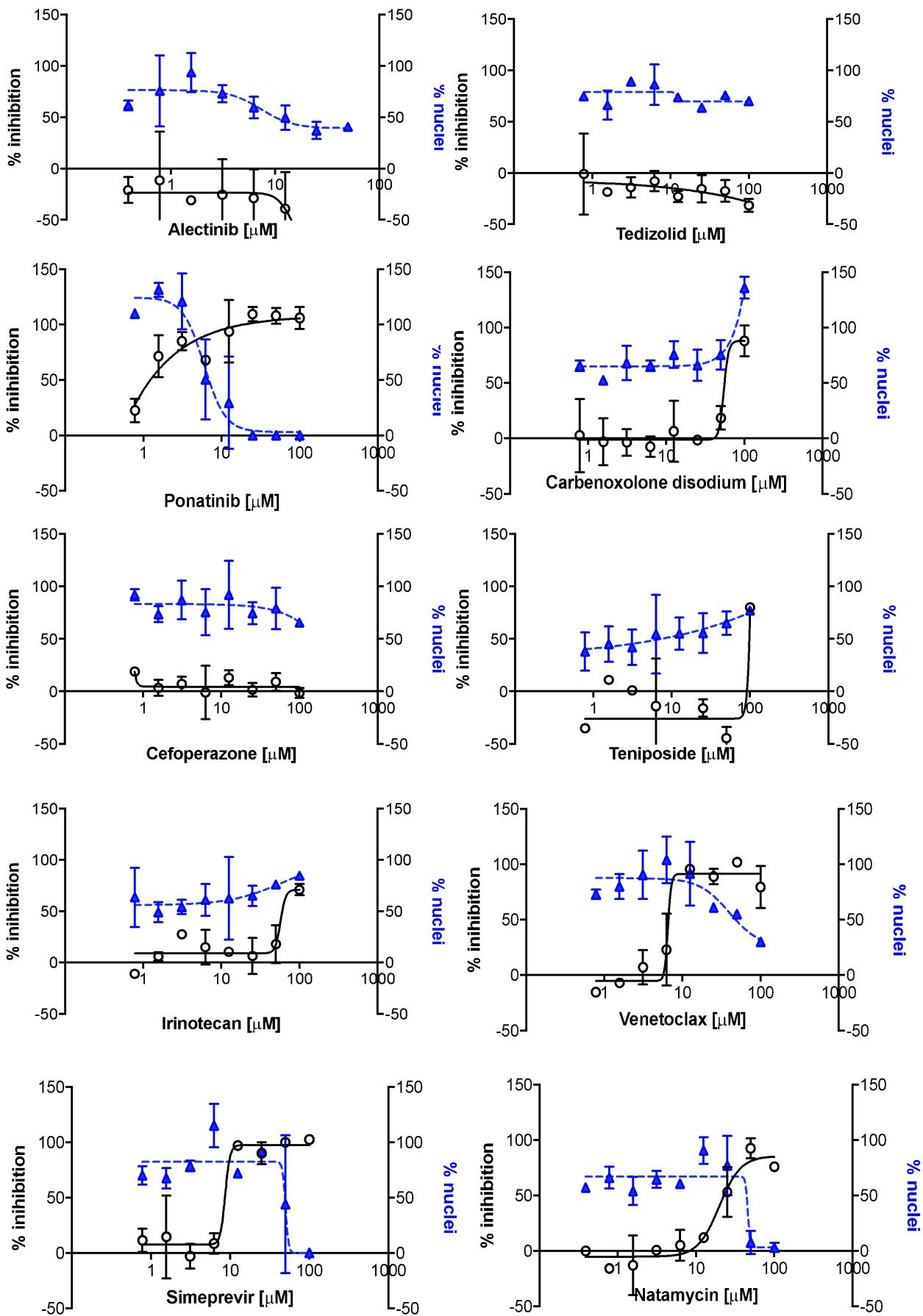
Combined *in silico* and *in vitro* approaches identified the antipsychotic drug lurasidone and the antiviral drug elbasvir as SARS-CoV2 and HCoV-OC43 inhibitors

Mario Milani, Manuela Donalisio, Rafaela Milan Bonotto, Edoardo Schneider, Irene Arduino, Francesco Boni, David Lembo, Alessandro Marcello *, Eloise Mastrangelo *

Table S1. List of the first best 60 compounds selected by *in silico* docking. In red the compounds selected for cell-based assays.

in silico ranking	Cpd	name	predicted ki [nM]
1	DB09534	Ecamsule	2.7
2	DB02633	Cibacron Blue	3.1
3	DB01830	AP-22408	4.2
4	DB01879	<i>experimental</i>	4.3
5	DB11363	Alectinib	8.5
6	DB04330	Bilh 434	12.2
7	DB09042	Tedizolid	20.2
8	DB03276	<i>experimental</i>	26.7
9	DB08901	Ponatinib	29.4
10	DB06581	Bevirimat	29.6
11	DB04016	<i>experimental</i>	30.0
12	DB02329	Carbenoxolone	34.8
13	DB08815	Lurasidone	64.3
14	DB08823	Spinosad	71.8
15	DB05340	ATL-2502	86.1
16	DB07189	<i>experimental</i>	110.2
17	DB09335	Alatrofloxacin	115.3
18	DB01329	Cefoperazone	115.7
19	DB01396	Digitoxin	148.6
20	DB03712	RU85053	164.9
21	DB11574	Elbasvir	167.6
22	DB06210	Eltrombopag	195.9
23	DB00444	Teniposide	204.3
24	DB11581	Venetoclax	208.4
25	DB09233	Cronidipine	212.8
26	DB02432	RU90395	216.7
27	DB00762	Irinotecan	247.6
28	DB01988	<i>experimental</i>	251.2
29	DB02169	<i>experimental</i>	259.4
30	DB04289	Genz-10850	279.2

in silico ranking	Cpd	name	predicted ki [nM]
31	DB07213	<i>experimental</i>	289.6
32	DB06290	Simeprevir	292.1
33	DB01836	<i>experimental</i>	376.4
34	DB05868	Ciluprevir	390.4
35	DB00511	Acetyl-digitoxin	416.1
36	DB09280	Lumacaftor	454.3
37	DB01251	Gliquidone	464.8
38	DB06925	<i>experimental</i>	485.7
39	DB04888	Bifeprunox	519.3
40	DB03957	SP2456	526.8
41	DB04881	Elacridar	527.0
42	DB08512	<i>experimental</i>	590.0
43	DB02112	Zk-806450	596.1
44	DB02194	<i>experimental</i>	602.5
45	DB04698	<i>experimental</i>	618.0
46	DB01267	Paliperidone	632.9
47	DB11575	Grazoprevir	639.9
48	DB00872	Conivaptan	696.8
49	DB04673	<i>experimental</i>	697.5
50	DB04877	Voacamine	709.5
51	DB07847	<i>experimental</i>	726.0
52	DB01897	<i>experimental</i>	740.9
53	DB03933	C-1027	799.3
54	DB00773	Etoposide	801.5
55	DB08164	<i>experimental</i>	803.0
56	DB08237	<i>experimental</i>	850.0
57	DB08676	<i>experimental</i>	855.5
58	DB00430	Cefpiramide	864.2
59	DB00826	Natamycin	945.3
60	DB01459	Bezitramide	953.5



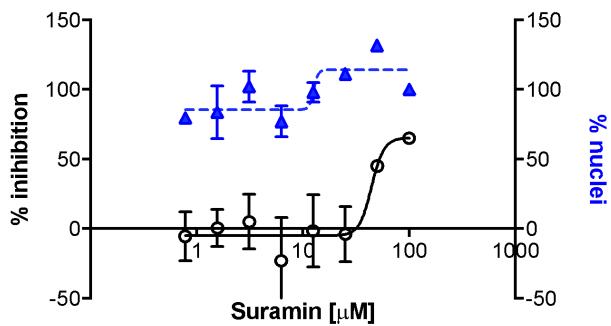
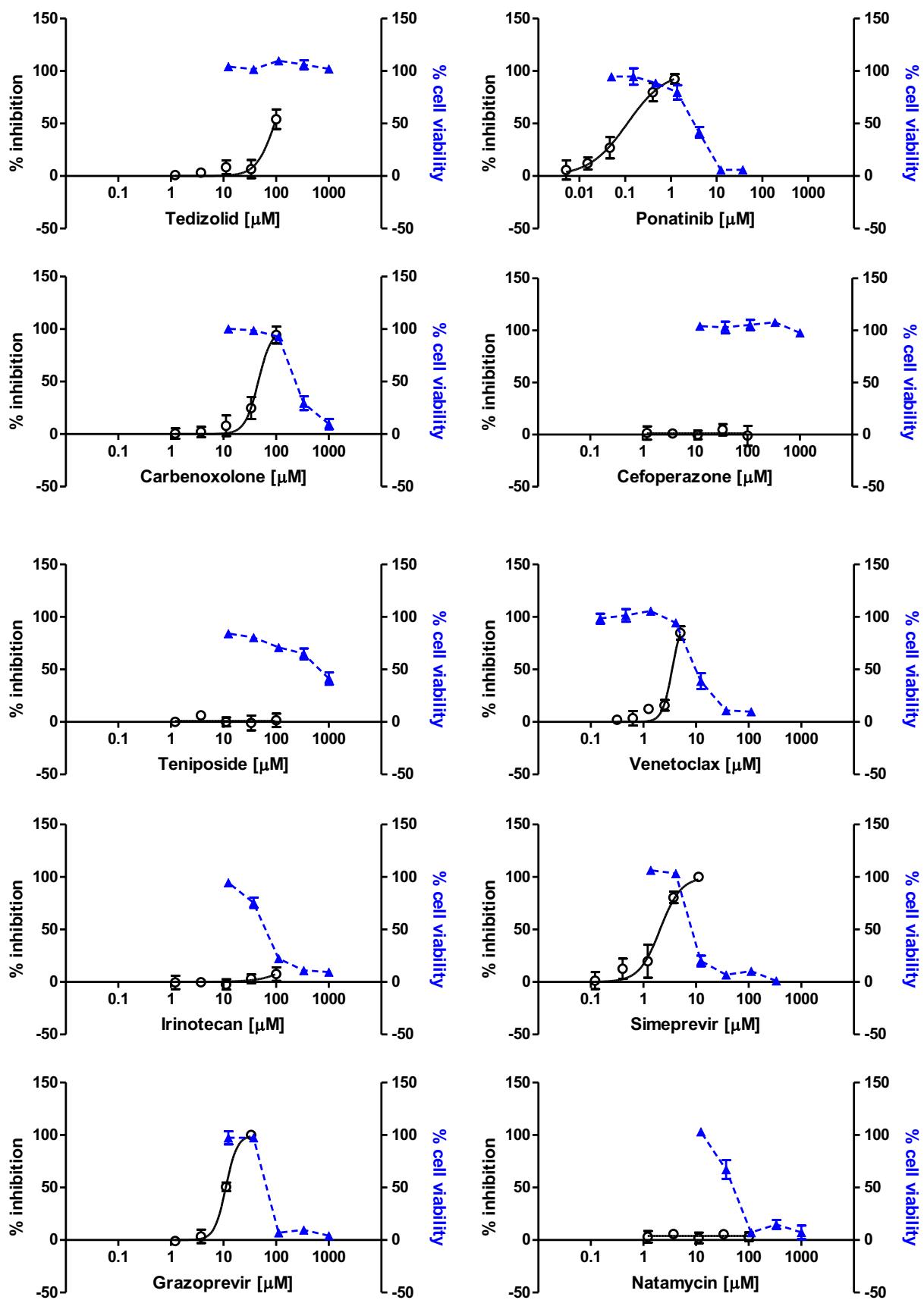


Figure S1: Antiviral efficacy of the selected compounds against SARS-CoV2. The antiviral activity of compounds was evaluated infecting Huh7-hACE2 cells in presence of increasing concentration of compounds. Number of nuclei were quantified in parallel. The percentage inhibition (white dots) was normalized with the average infection ratio of wells treated with 1% DMSO. Percentage of nuclei (blue triangles) was calculated by comparing the average number of nuclei of non-infected wells treated with 1% DMSO. Error bars represent the standard deviation (SD) of 2 independent experiments.



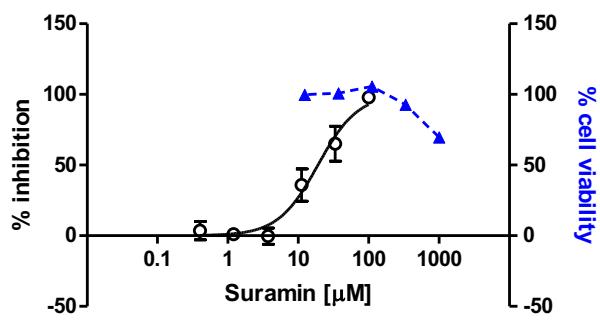


Figure S2: Antiviral efficacy of the selected compounds against HCoV-OC43. The antiviral activity of compounds was evaluated infecting MRC-5 cells in presence of increasing concentration of compounds. Cell viability assays were performed in the same conditions as for antiviral assays, in absence of viral inoculum. The percentage inhibition (white dots) and the percentage of cell viability (blue triangles) were calculated by comparing treated and untreated wells. Error bars represent the standard deviation (SD) of 3 independent experiments.