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In Vitro and *In Silico* Studies of *Bis*-furyl-pyrrolo[3,4-*b*]pyridin-5-ones on Dengue Virus

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Supplementary Information

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***In vitro* assays**

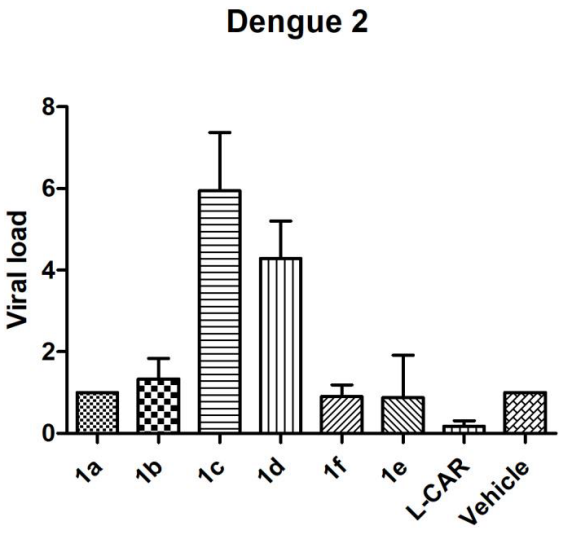

Fig. S1. Inhibition of DENV serotype 2 infection in Vero CCL-81 cells.

Docking
Cartesian coordinates of bioactive conformations
Pose of 1a into NS3

C	46.41810	-3.61050	1.18870
C	46.00310	-2.28890	1.08990
C	46.24750	-1.55070	-0.01810
N	46.90050	-2.07240	-1.08560
C	47.33180	-3.37060	-1.06630
C	47.09770	-4.17940	0.08420
C	45.31480	-1.42890	2.01660
C	45.71340	-0.16050	0.12660
H	46.22220	-4.17400	2.09110
C	48.07120	-3.89130	-2.27180
N	47.56260	-5.54780	0.10870
C	46.45850	-6.50470	0.28750
C	48.60430	-5.75170	1.12750
H	45.72570	-6.39800	-0.54100
H	45.93030	-6.33680	1.25220
C	47.02240	-7.92980	0.27430
H	47.45510	-8.16820	-0.72410
H	46.19200	-8.64460	0.45410
O	47.98860	-8.09450	1.29640
C	49.07410	-7.21070	1.08200
H	49.47130	-5.08720	0.91790
H	49.57690	-7.42760	0.11200
H	49.82370	-7.36990	1.88550
H	48.16020	-3.06120	-3.00550

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H	48.85990	-6.52020	-2.37940
H	49.10650	-4.20890	-2.02790
C	47.33810	-5.05950	-2.87660
C	46.08450	-4.86900	-3.48240
C	45.40270	-5.95080	-4.04770
C	45.96490	-7.22960	-4.01080
C	47.20960	-7.42870	-3.40740
C	47.89490	-6.34960	-2.84040
H	45.63720	-3.88450	-3.51540
H	44.43800	-5.79770	-4.51400
H	45.43590	-8.06610	-4.44910
H	47.64390	-8.41970	-3.37930
O	45.00500	-1.75790	3.15170
N	45.09990	-0.09910	1.48740
C	43.65680	0.20080	1.40670
C	43.94190	2.66210	1.69720
C	46.82010	0.85330	0.01300
O	42.44990	1.65520	3.08700
H	49.69320	2.25810	0.61540
H	41.94670	3.49510	4.12420
H	44.68810	2.79920	0.92110
C	42.53140	3.01110	3.34910
C	43.38590	3.65870	2.57140
H	43.61180	4.71930	2.60020
H	43.05120	-0.60110	1.88810
H	43.34180	0.26920	0.34140
C	43.35490	1.52510	2.04840
H	44.97440	0.01430	-0.68890
H	48.22620	0.07000	1.45940
O	46.75250	1.91570	-0.87140
C	47.96450	2.54110	-0.64030
C	48.71090	1.94570	0.27720
H	48.27160	3.43820	-1.16740
C	47.94670	0.81090	0.71720
H	48.22000	-5.52650	2.14750

Pose of 1a into NS3-2B

C	28.11440	-0.99740	60.55440
C	28.46810	-2.31290	60.28440
C	29.65440	-2.62400	59.71140
N	30.55480	-1.66480	59.38400
C	30.28140	-0.34670	59.62810
C	29.04080	0.02210	60.22620
C	27.76490	-3.55360	60.48000
C	29.79160	-4.10090	59.51420
H	27.15420	-0.77500	61.00020
C	31.30930	0.67850	59.22390
N	28.74760	1.41550	60.47440
C	28.02260	2.03700	59.35430
C	29.96230	2.17850	60.80160
H	27.06410	1.50270	59.17930
H	28.62240	2.00600	58.41770
C	27.72240	3.49960	59.70060
H	27.02520	3.55940	60.56730

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H	27.21550	3.97530	58.83480
O	28.92040	4.20640	59.96600
C	29.58040	3.63690	61.08200
H	30.44260	1.75090	61.70910
H	28.94600	3.70450	61.99510
H	30.50620	4.21710	61.27930
H	31.39420	1.42250	60.04540
H	29.58260	-0.24040	57.29560
H	32.31900	0.23600	59.09360
C	30.90730	1.35020	57.93740
C	31.43470	2.60920	57.60380
C	31.06600	3.23420	56.40870
C	30.16770	2.60920	55.53970
C	29.63570	1.35850	55.86510
C	30.00140	0.73000	57.05970
H	32.12910	3.10490	58.26910
H	31.47640	4.20340	56.15650
H	29.88340	3.09420	54.61470
H	28.93980	0.87560	55.19130
O	26.62560	-3.63110	60.91430
N	28.52370	-4.70050	60.02880
C	28.78870	-5.62200	61.15100
C	31.13960	-6.39520	61.46640
C	29.96540	-4.43300	58.05640
O	30.63090	-4.35500	62.33260
H	31.39810	-4.51940	55.13570
H	32.62750	-4.02470	63.11930
H	31.03080	-7.35100	60.96380
C	31.95270	-4.68040	62.57920
C	32.31450	-5.86050	62.09900
H	33.29520	-6.31790	62.17610
H	28.59890	-6.67990	60.85690
H	28.11720	-5.38290	62.00590
C	30.20230	-5.47160	61.63690
H	30.69090	-4.44410	60.07540
H	31.86220	-3.47240	57.65370
O	29.03800	-5.18990	57.36190
C	29.61630	-5.24610	56.10650
C	30.77160	-4.60510	56.01710
H	29.16060	-5.77110	55.27370
C	31.01030	-4.05900	57.32480
H	30.69390	2.15030	59.96330