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Identification of Novel Non-Nucleoside Inhibitors of Zika Virus NS5 Protein Targeting MTase Activity

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Table of Contents

Figure S1 3
Figure S2 4
Figure S3 4
Table S1 5

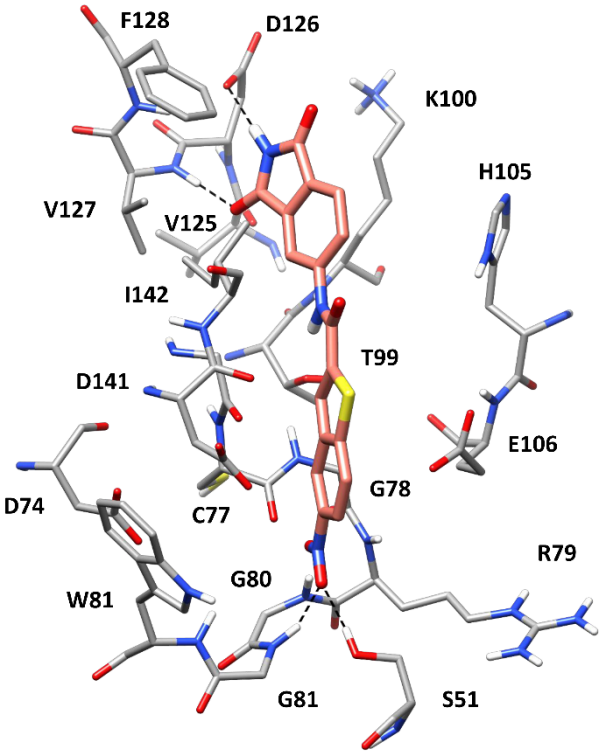


Figure S1. Binding mode of ligand 1 predicted by docking. The hydrogen bonds corresponding to the required pharmacophore features are shown as black dashed lines.

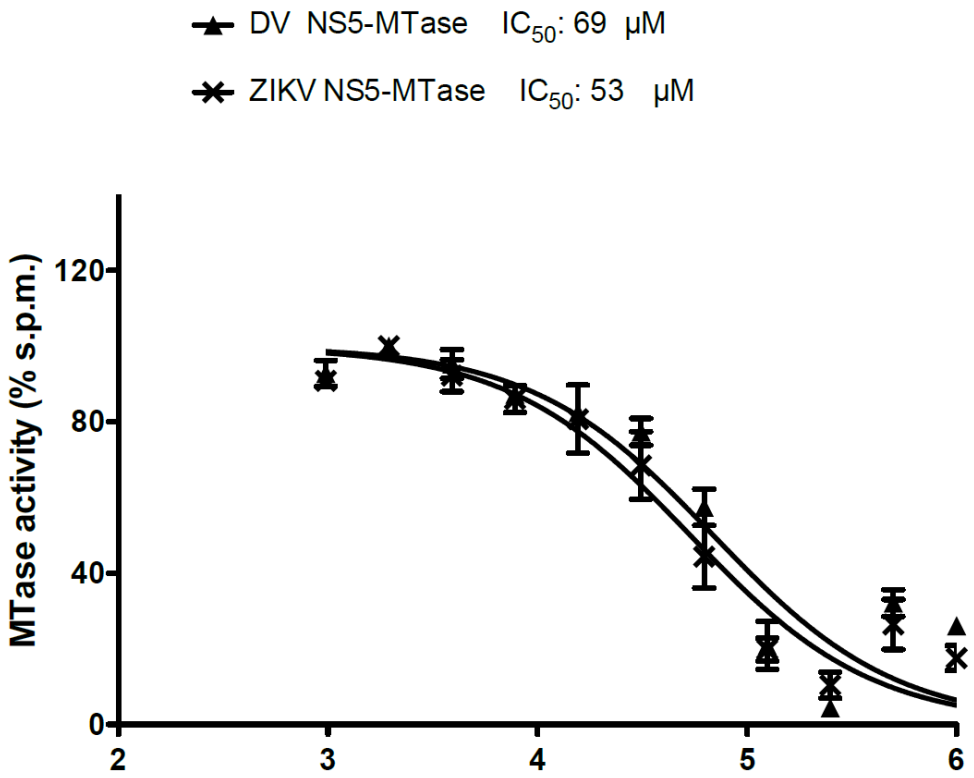


Figure S2. Inhibitory curves for compound **1** vs Dengue (DV) and Zika (ZIKV) virus methyltransferase (Mtase) and IC50 values.

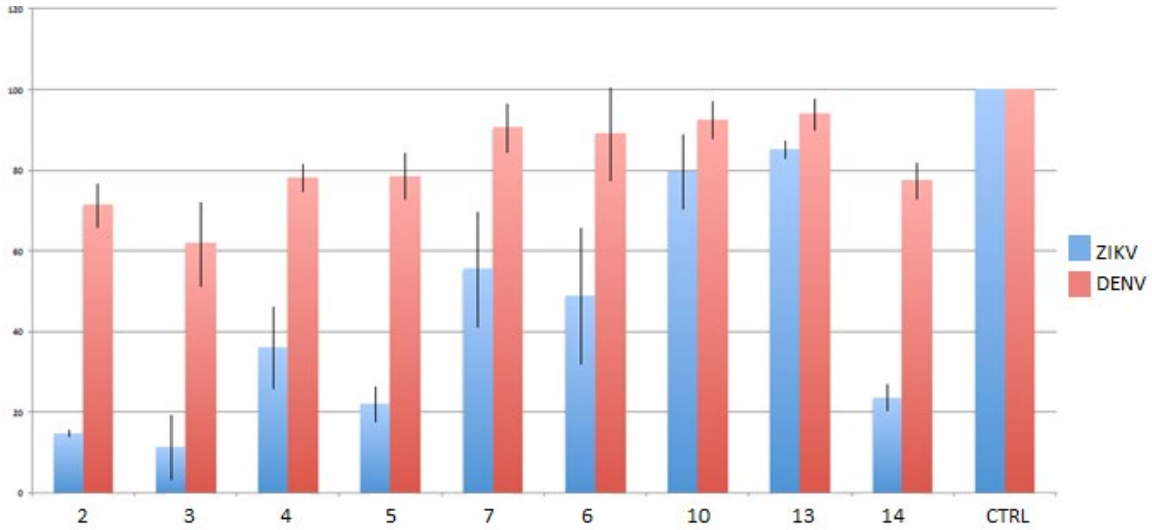


Figure S3. Screening of compounds against ZIKV and DENV N-terminal methyltransferase (Mtase). Only representative compounds are shown.

Table S1. Molecular mechanics-generalized Born surface area (MM-GBSA) values calculated for compounds **1**–**20**.

Compound ID	MMGBSA (kcal/mol)	StDev
1	-32.0	4.3
2	-33.9	5.1
3	-36.2	4.9
4	-21.7	3.9
5	-23.4	4.5
6	-29.8	4.0
7	-18.2	4.5
8	-28.3	3.9
9	-17.8	4.1
10	-30.7	3.4
11	-22.3	3.7
12	-21.6	3.6
13	-29.4	4.8
14	-26.2	3.1
15	-26.4	3.9
16	-26.7	4.0
17	-28.6	4.1
18	-25.2	4.4
19	-28.3	3.7
20	-28.8	3.2