

Supporting Information

Thioguanine-based DENV-2 NS2B/NS3 protease inhibitors: Virtual screening, synthesis, biological evaluation and molecular modelling

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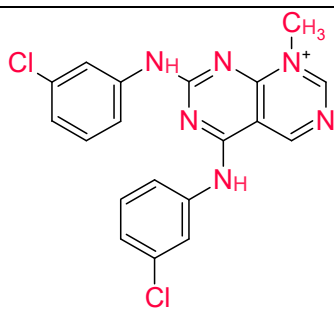
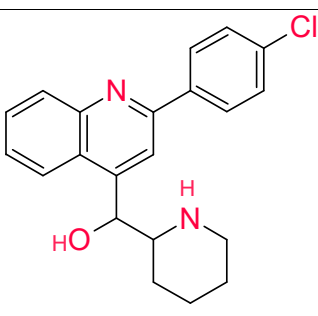
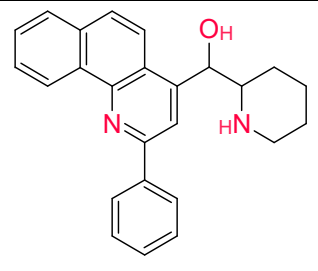
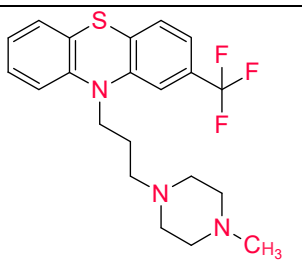
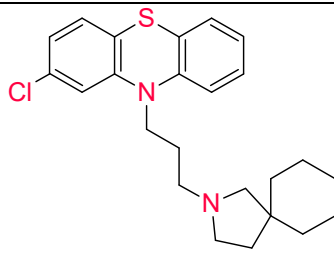
⁹School of Data Sciences, Perdana University, Blok B and d1, MAEPS Building, MARDI Complex, Jalan MAEPS Perdana, 43400 Serdang, Selangor

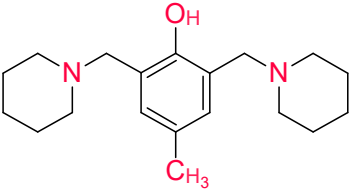
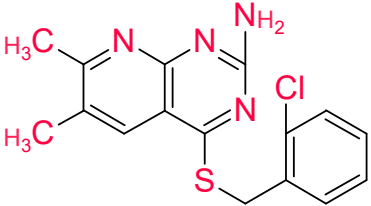
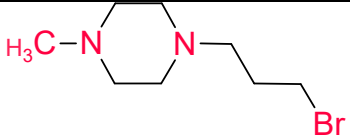
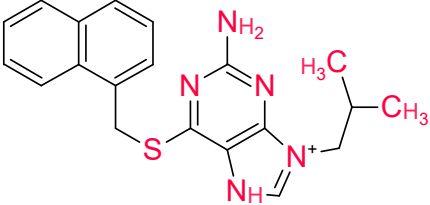
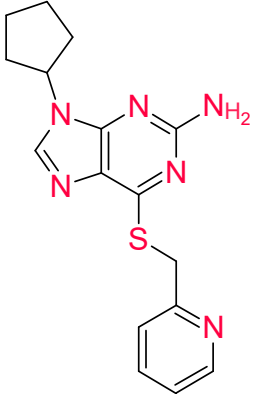
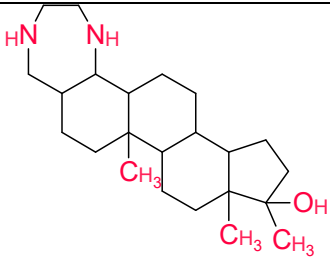
* Corresponding Author

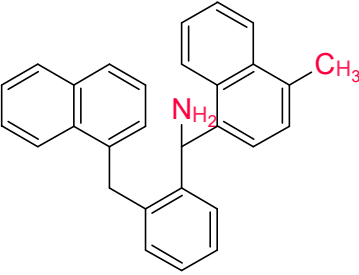
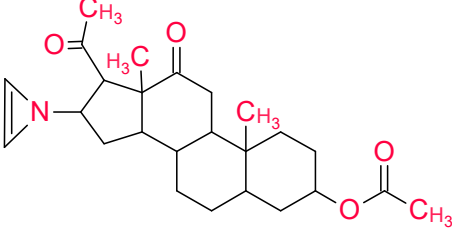
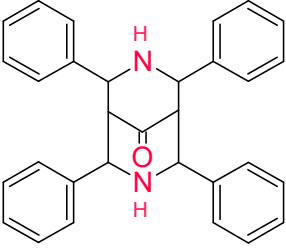
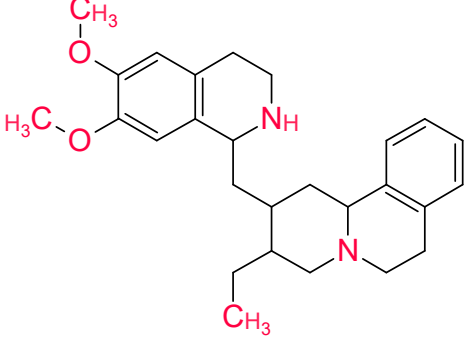
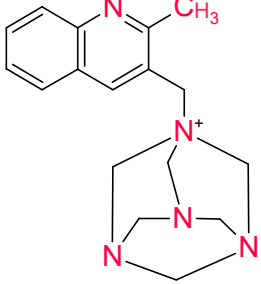
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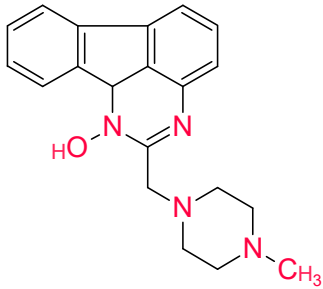
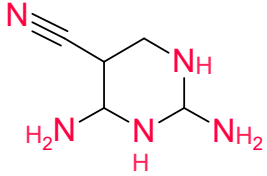
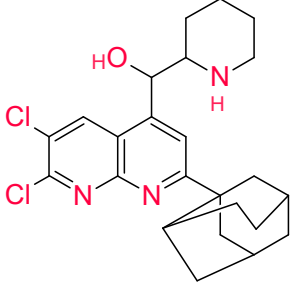
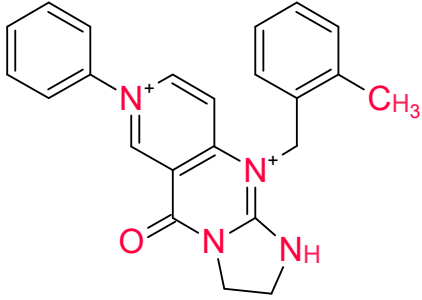
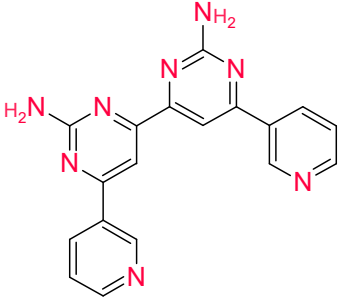
&These authors contributed equally to this work

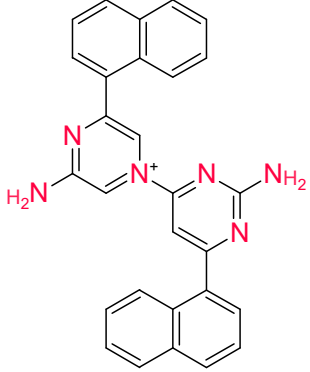
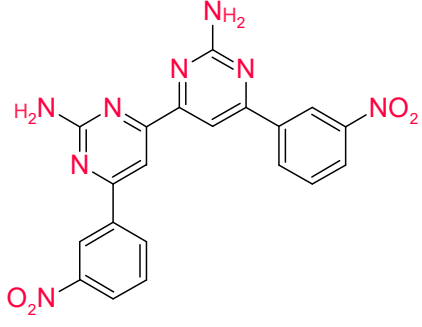
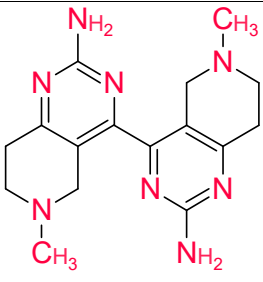
S1 Table

Compounds	Structures	ΔG_{bind} (kcal/mol)
NSC11668 (D0126)		-7.9
NSC13316 (D0152)		-6.8
NSC13480		-7.8
NSC17474 (D0227)		-6.9
NSC19976 (D0265)		-6.5

NSC37881		-5.8
NSC54278		-7.6
NSC54970		-3.9
NSC56452 (D0685)		-7.3
NSC59486 (D0713)		-7.1
NSC116977		-7.1

NSC99504		-7.6
NSC118208		-7.0
NSC122140		-7.2
NSC47704		-7.0
NSC34924		-6.6

<p>NSC170561 (D1498)</p>		<p>-7.4</p>
<p>NSC211322</p>		<p>-5.3</p>
<p>NSC48874</p>		<p>-7.3</p>
<p>NSC350625 (D1804)</p>		<p>-7.3</p>
<p>NSC371872</p>		<p>-8.4</p>

<p>NSC371876 (D1853)</p>		<p>-9.9</p>
<p>NSC371880 (D1855)</p>		<p>-8.9</p>
<p>NSC372037</p>		<p>-8.3</p>