SUPPLEMENTARY MATERIAL

Expanding the Structural Diversity of DNA Methyltransferase Inhibitors

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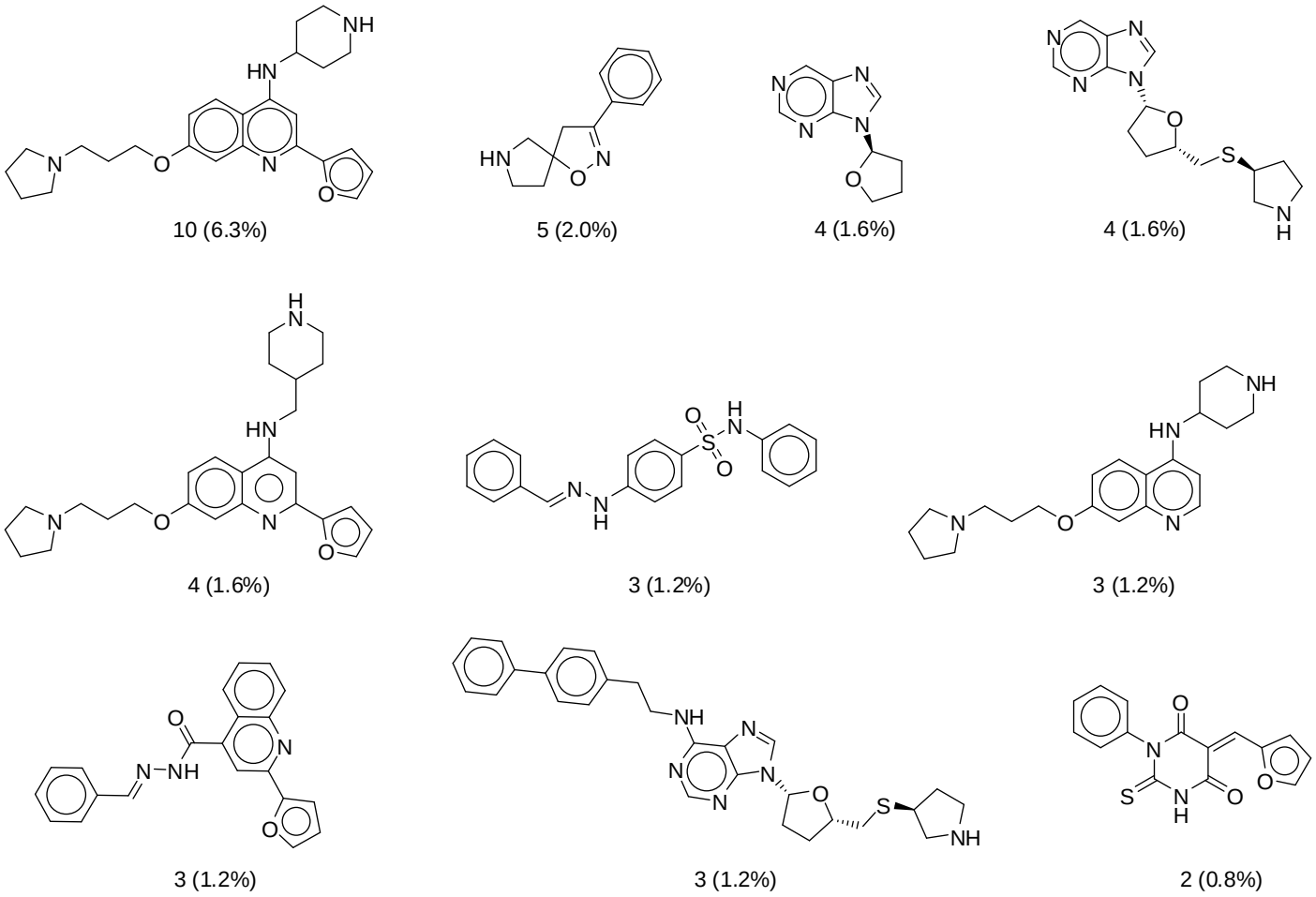
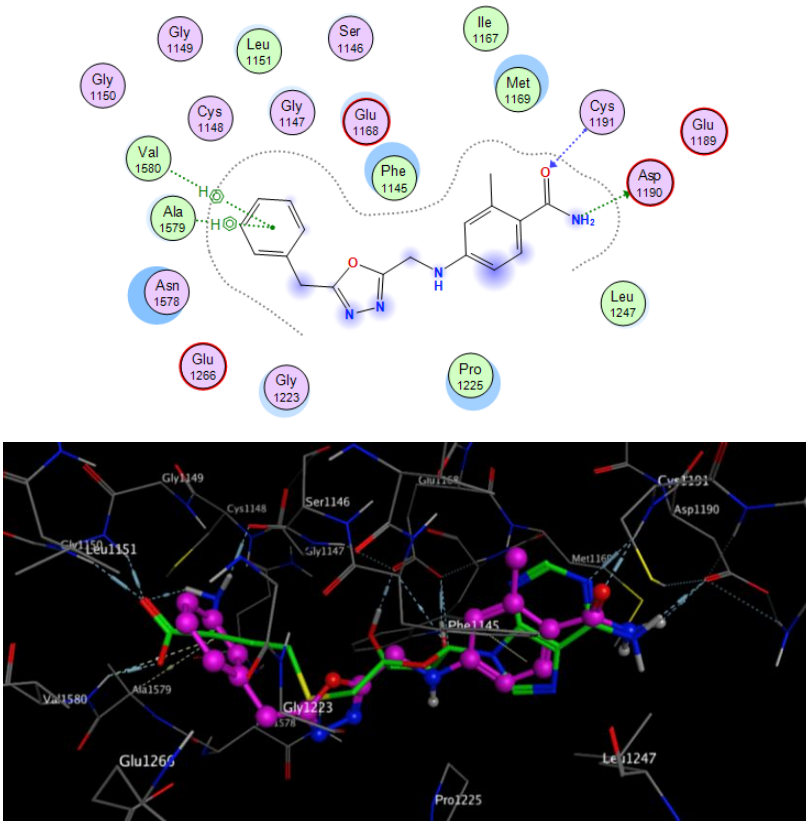


Figure S1. Chemical structures of the ten most frequent (Bemis-Murcko) scaffolds of the active DNMT inhibitors available in ChEMBL 27. The percentage of frequency is indicated in parenthesis.

Table S1. Chemical vendors of the ten compounds tested and their purity as supplied by the vendor.

Compound	Vendor	Purity % (provided by vendor)
Glyburide	TargetMol	99.77
Panobinostat	TargetMol	98
Theaflavin	TargetMol	97.76
7936171	Chembridge	>=90
CSC027480404	ChemSpace	90
CSC026286840	ChemSpace	100
CSC027694519	ChemSpace	100
6631802	Chembridge	>=90
CSC027796832	ChemSpace	94
CSC027083851	ChemSpace	100

A



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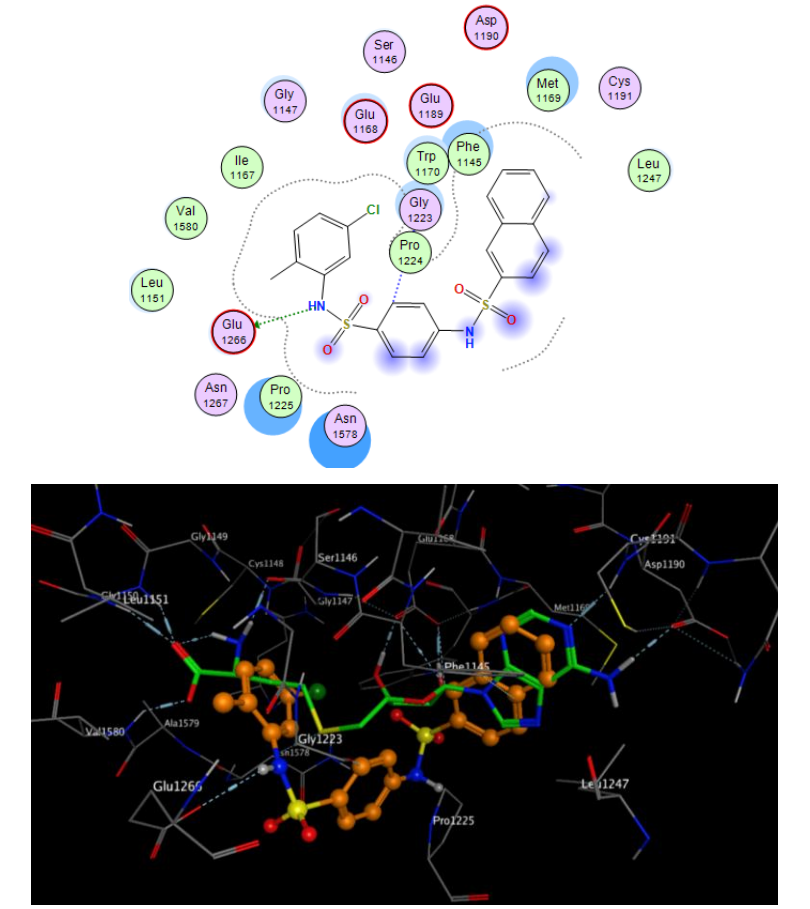

Figure S2. Comparison of the co-crystal position of SAH in the catalytic site of DNMT1 (PDB ID: 4WXX) with the predicted binding mode of **A**) **CSC027694519** and **B**) **7936171**.

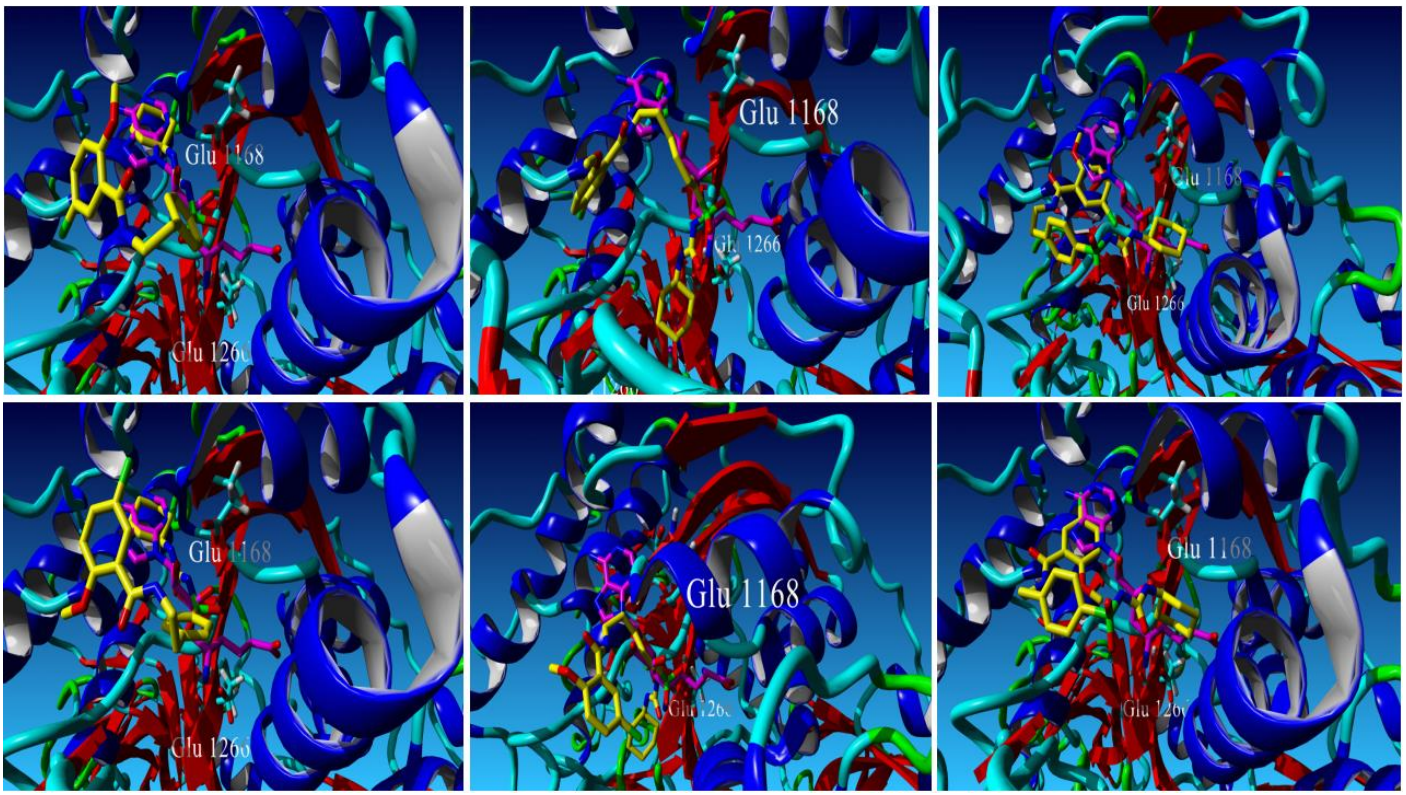

Figure S3. Docking poses of glyburide with DNMT1 obtained with the software PLANTS.

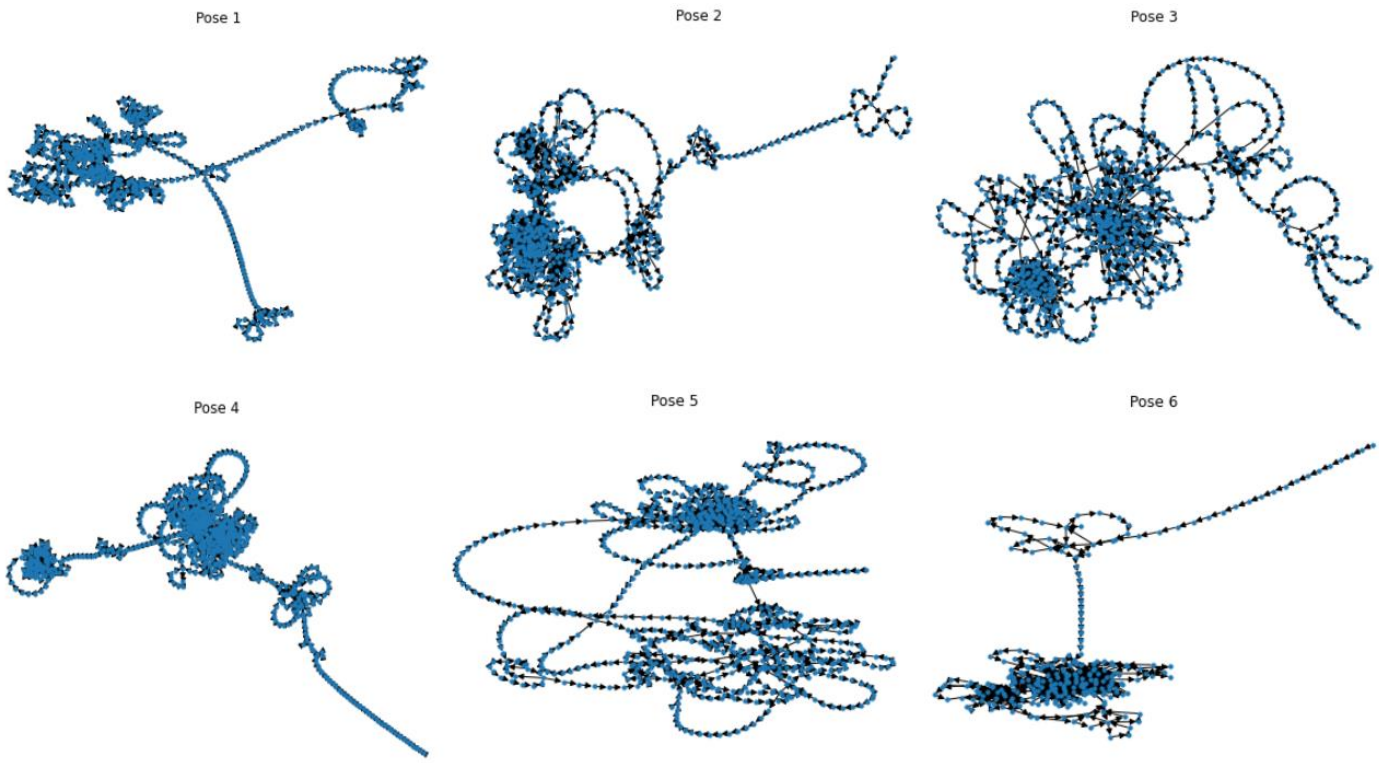

Figure S4. Microstate network analysis of glyburide.