Supplementary Material: *In Silico* Exploration of 1,7-Diazacarbazole Analogs As Checkpoint Kinase 1 Inhibitors By Using 3D QSAR, Molecular Docking Study, and Molecular Dynamics Simulations

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The structure of all the aligned molecular dataset used for the 3D QSAR studies were shown in Figure 1A. The 3D structures of the studies molecules were drawn and the 3D-QSAR studies were performed in SYBYL-X 2.0.

Table S1. Chemical structural formulas of all structures.

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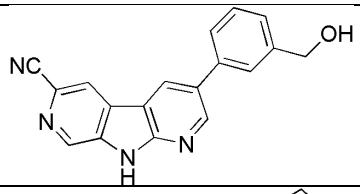
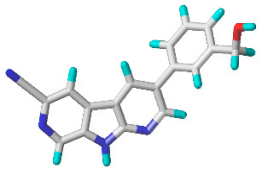
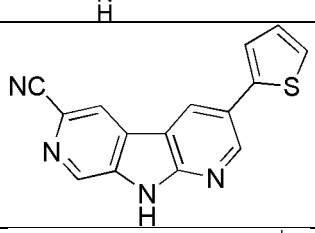
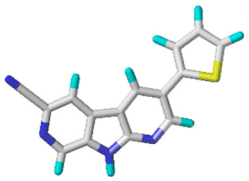
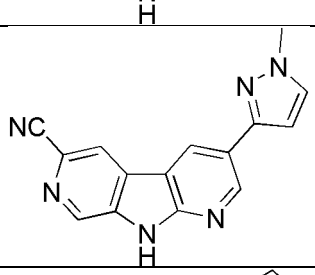
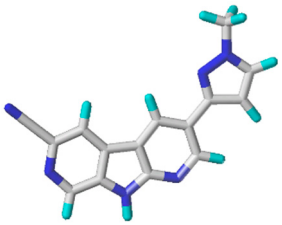
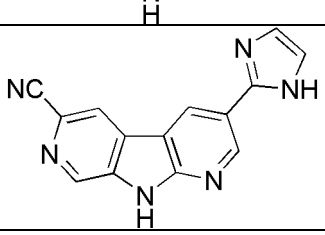
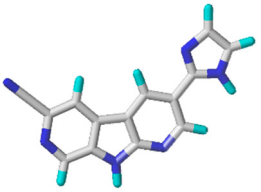
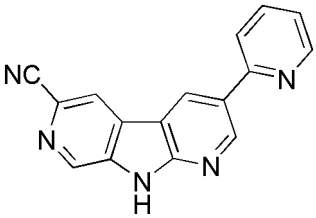
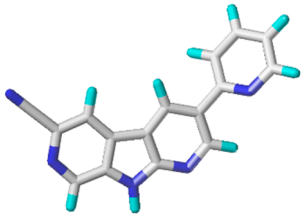
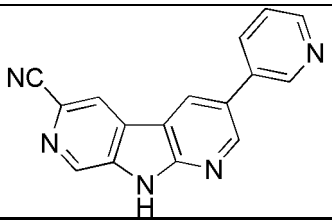
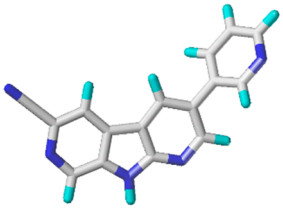
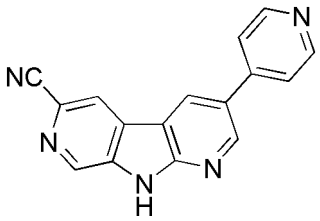
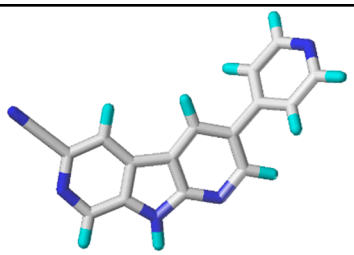
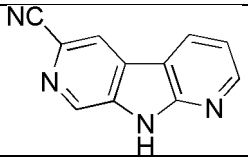
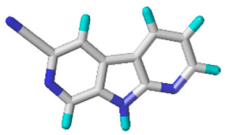
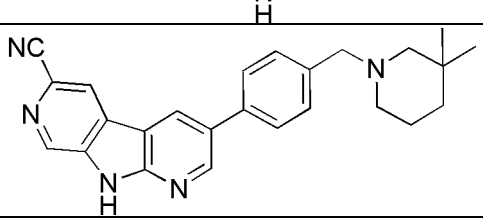
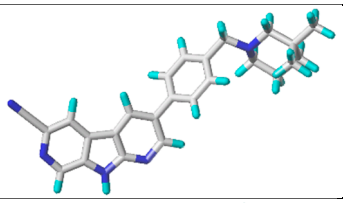
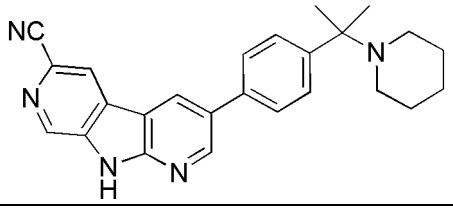
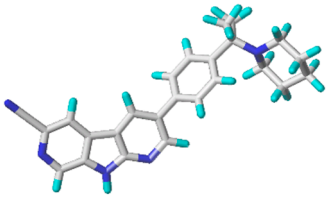
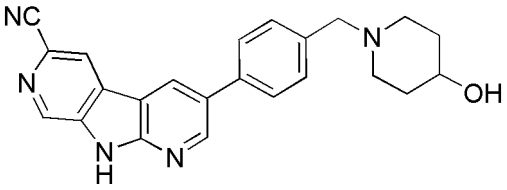
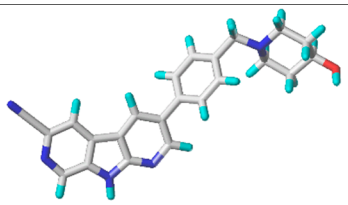
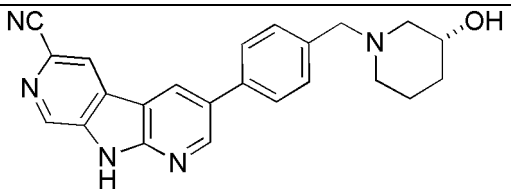
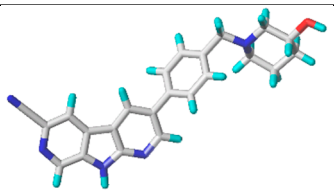
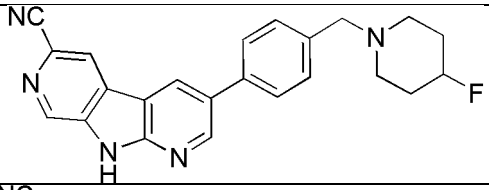
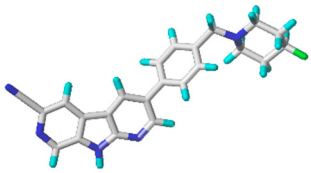
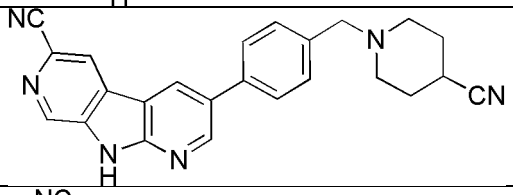
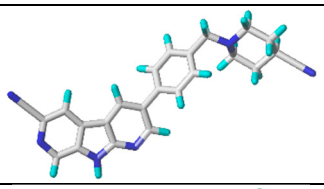
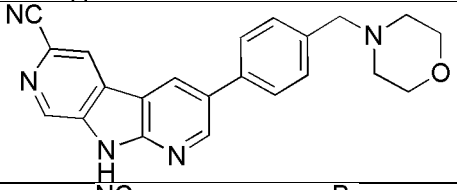
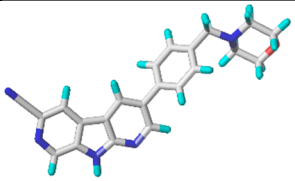
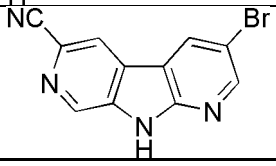
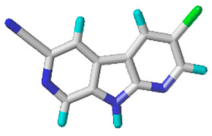
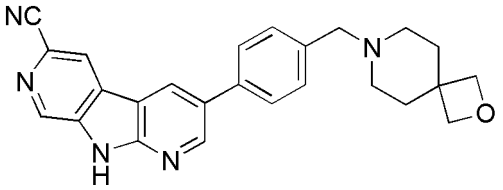
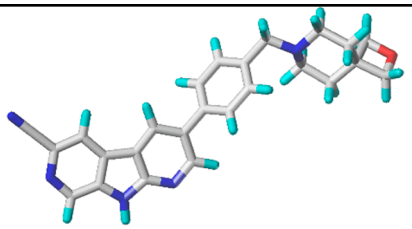
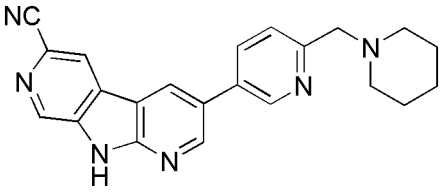
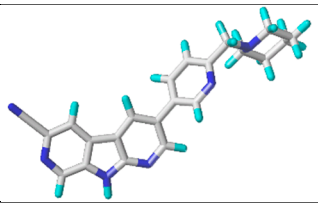
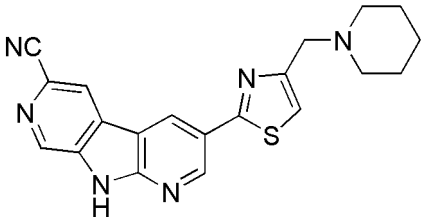
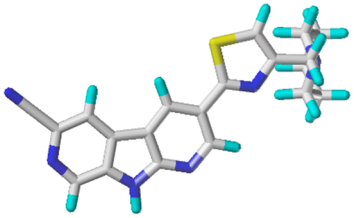
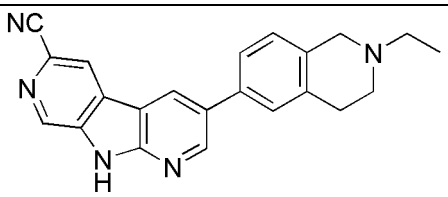
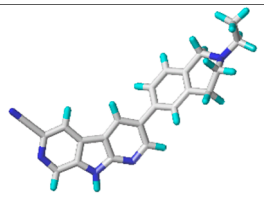
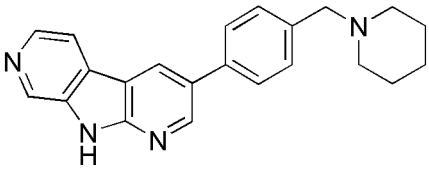
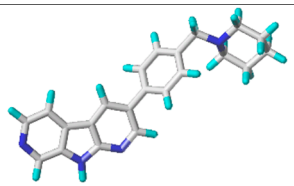
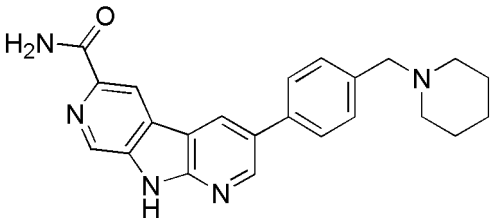
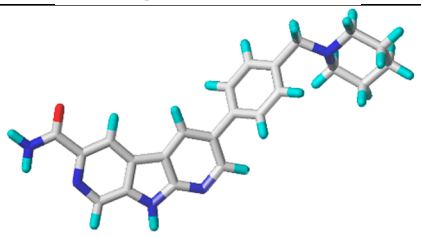
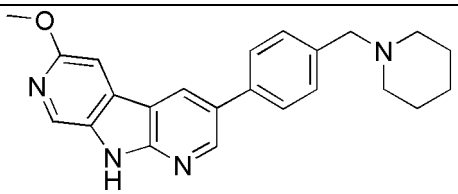
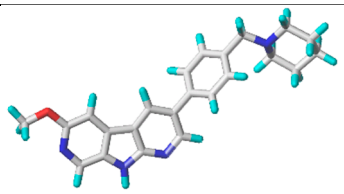
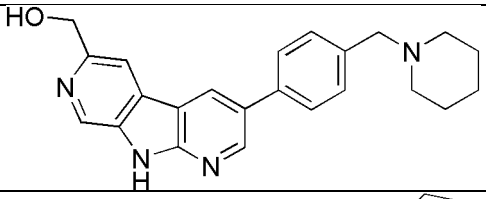
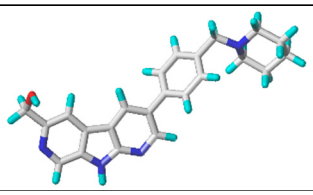
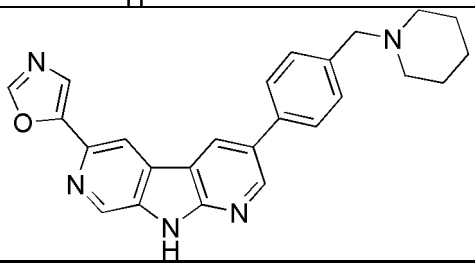
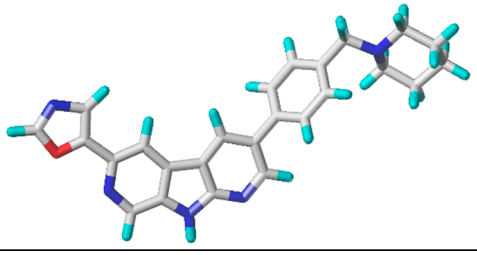
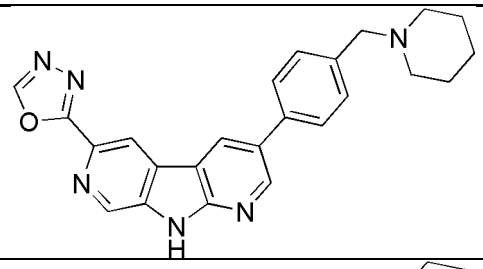
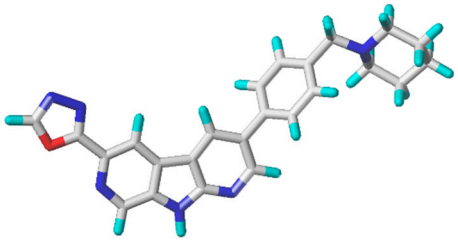
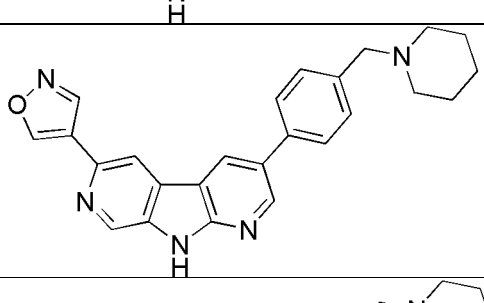
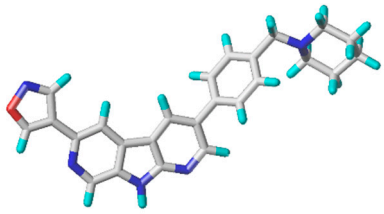
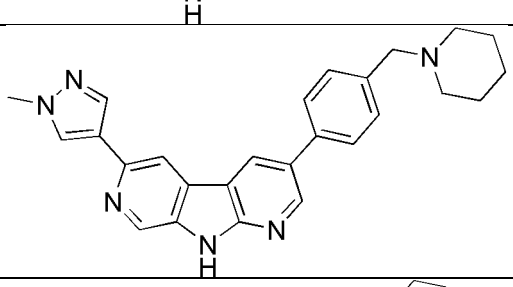
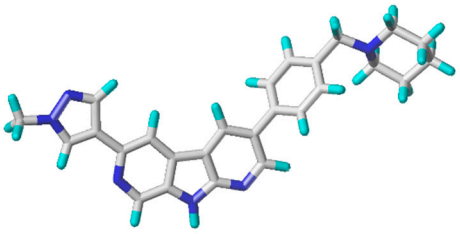
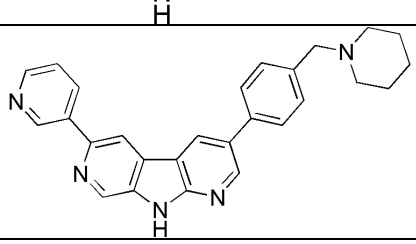
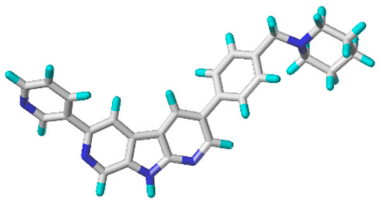
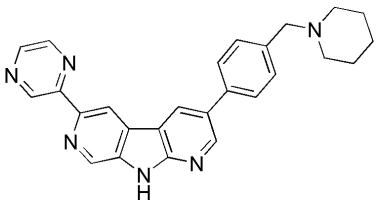
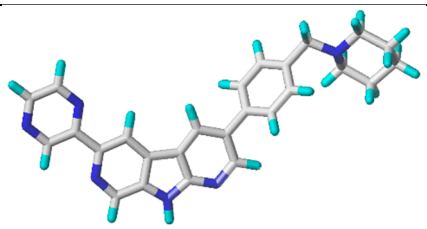
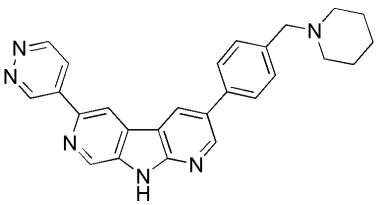
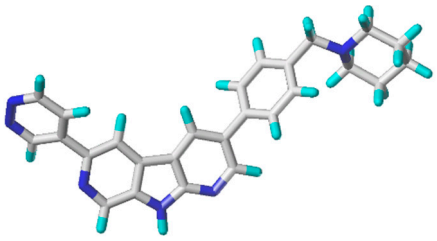
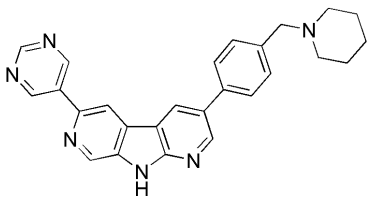
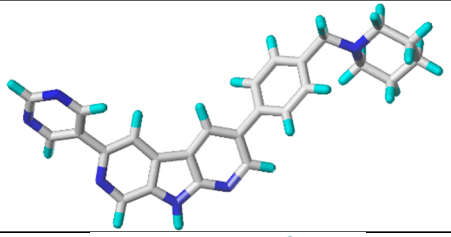
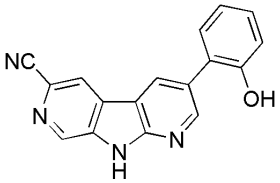
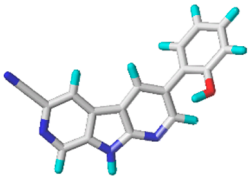
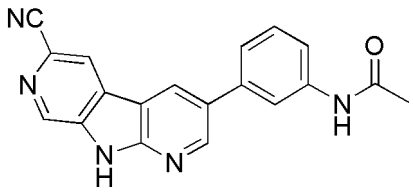
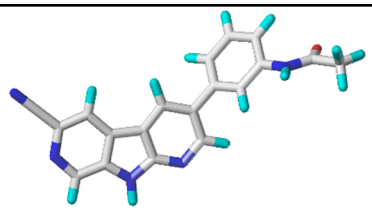
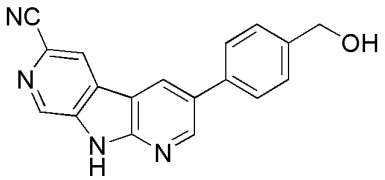
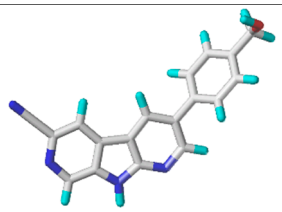
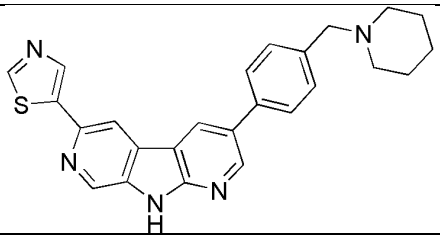
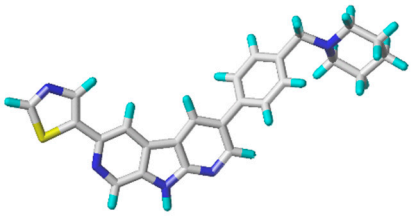
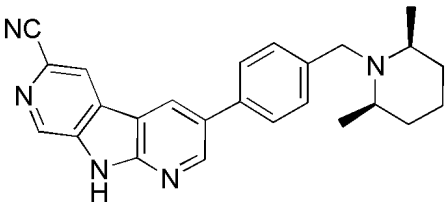
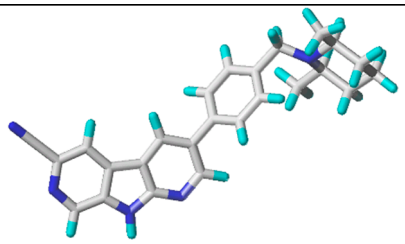
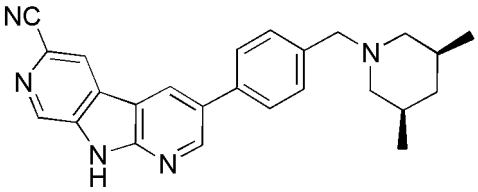
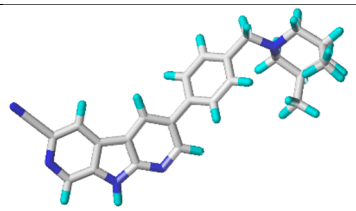
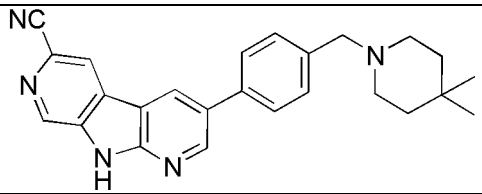
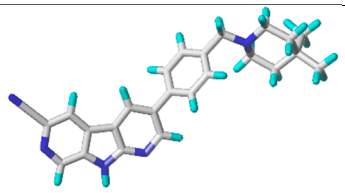
1		
2		
3		
4		
5		
6		

7		
8		
9		
10		
11		
12		
13		
14		
15		
16		

17		
18		
19		
20		
21		
22		
23		
24		
25		

26		
27		
28		
29		
30		
31		
32		
33		

34		
35		
Test1		
Test2		
Test3		
Test4		
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