Supplementary Materials: An Investigation of Molecular Docking and Molecular Dynamic Simulation on Imidazopyridines as B-Raf Kinase Inhibitors

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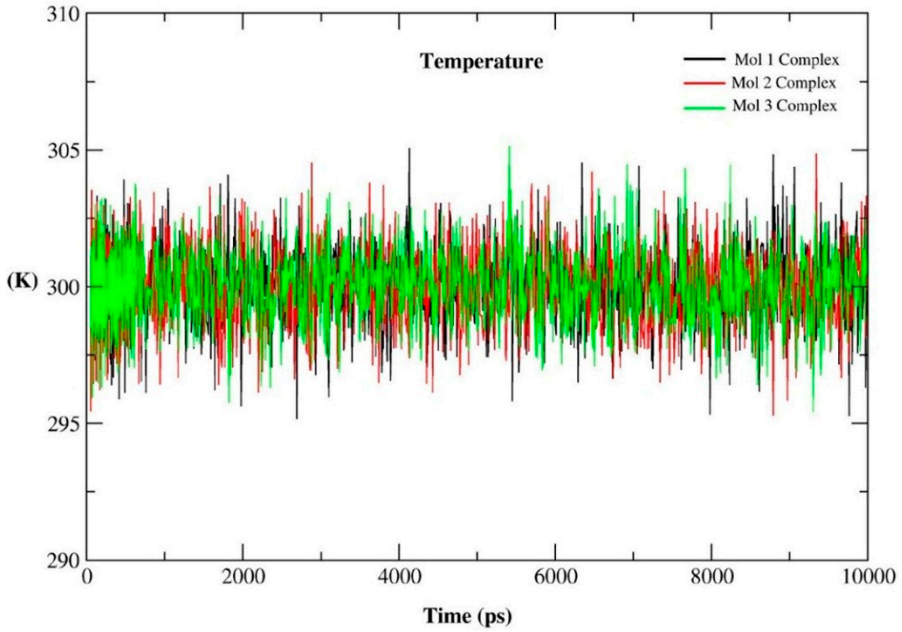


Figure S1. The temperature fluctuation *versus* time.

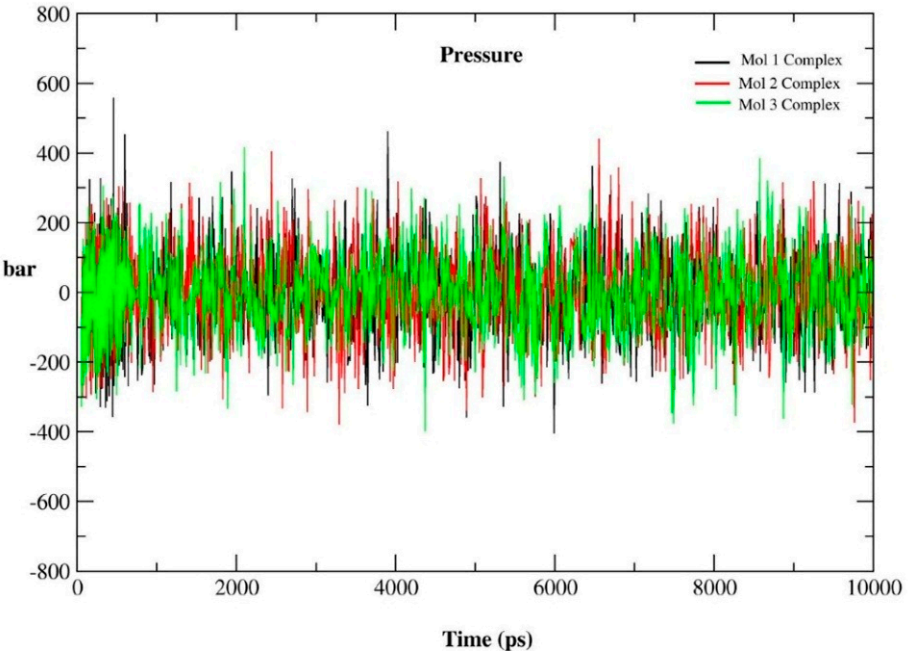


Figure S2. The pressure fluctuation *versus* time.

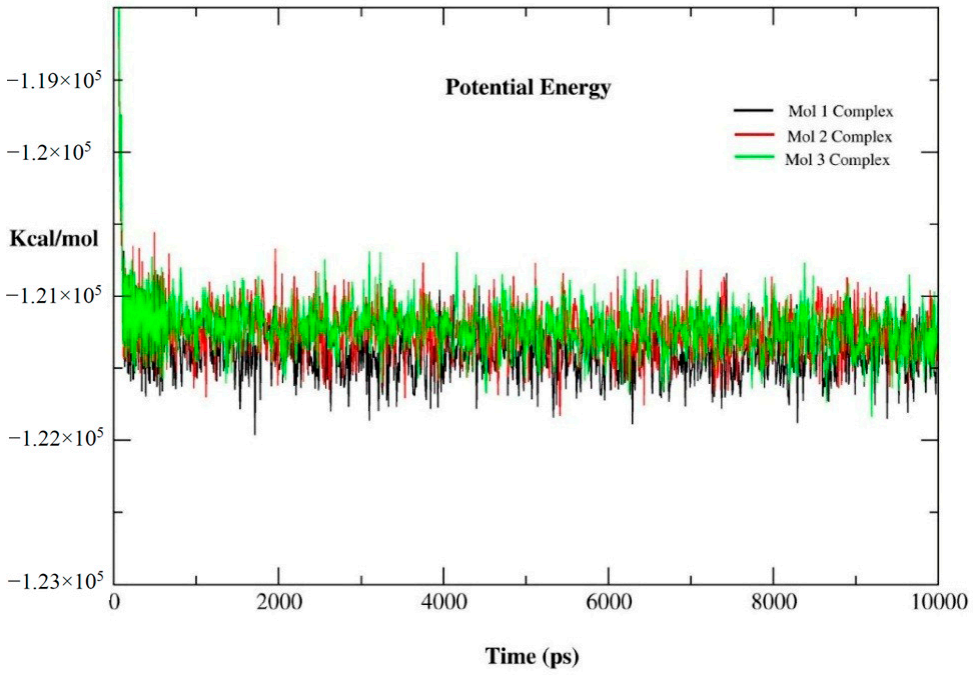
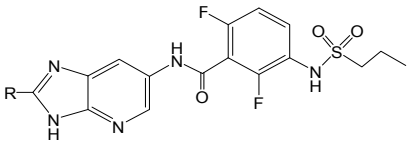
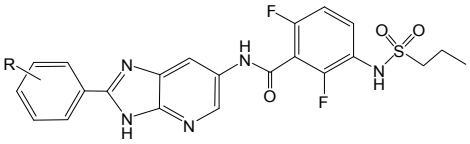
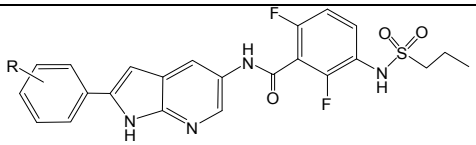
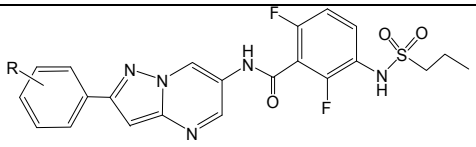


Figure S3. The potential energy fluctuation *versus* time.

Table S1. Chemical structures, biological activity values, and docking C_scores of the imidazopyridines.

Compound	General Structure	Substituent	IC_{50} (nM)	pIC_{50}	C_Score
1 (Mol 1)		H	61	7.215	6.37
2		Me	40	7.398	7.27
3		Et	59	7.229	5.97
4		*i*-Pr	60	7.222	7.13
5		*t*-Bu	69	7.161	7.07
6		Cyclobutyl	31	7.509	5.98
7		4-Piperidine	107	6.971	7.22
8 (Mol 3)		3-Piperidine	167	6.777	7.56
9		H	3.6	8.444	7.62
10		4-F	4.4	8.357	9.57
11		4-Cl	2.2	8.658	9.56
12		4-Br	2.2	8.658	9.48
13		3-F	3.1	8.509	9.53
14		3-Cl	1.1	8.959	9.71
15 (Mol 2)		3-Br	0.76	9.119	9.74
16		2-F	8.0	8.097	9.20
17		2-Cl	27	7.569	7.38
18		2-Br	27	7.569	7.42
19		3,4-di-F	3.4	8.469	8.32
20		3,4-di-Cl	1.5	8.824	8.54
21		4-MeO	1.1	8.959	7.85
22		4-Me	1.3	8.886	9.51
23		4-CF_3	1.4	8.854	8.25
24		4-CF_3O	2.4	8.62	7.95
25		4-CN	2.7	8.569	8.18
26		4-$MeSO_2$	1.4	8.854	8.01
27		3-MeO	1.2	8.921	9.42
28		3-CF_3	1.0	9.000	8.79
29		4-Pyridyl	3.2	8.495	7.74
30		3-Pyridyl	3.0	8.523	9.39
31		H	1.0	9.000	8.19
32		4-F	1.1	8.959	6.71
33		4-Cl	2.4	8.62	8.38
34		H	4.6	8.337	6.13
35		4-F	11	7.959	4.77
36		4-Cl	8.2	8.086	5.30