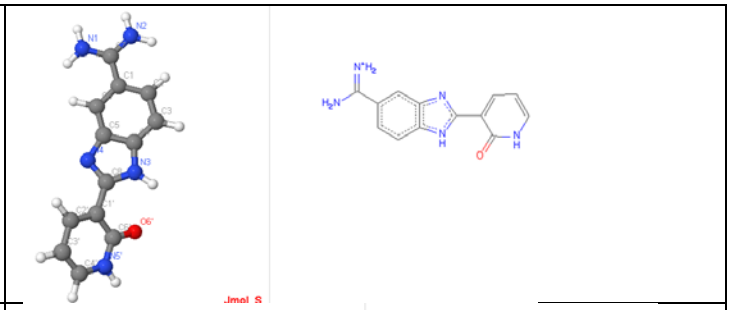
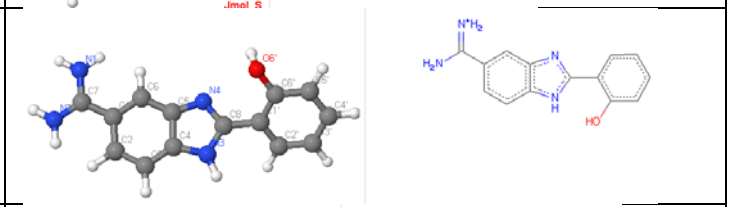
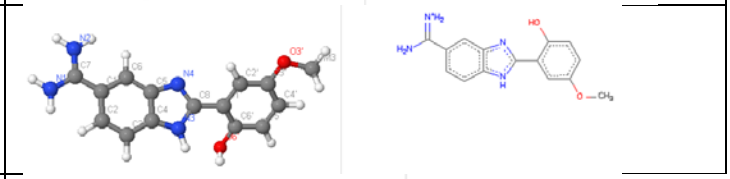
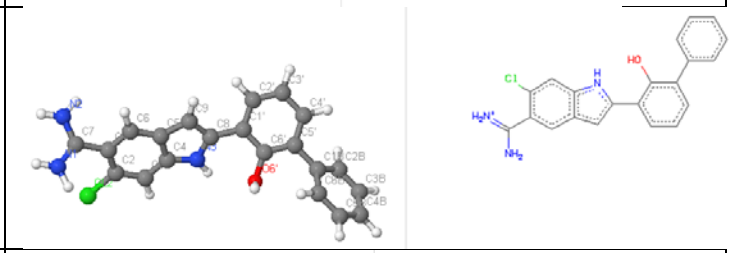
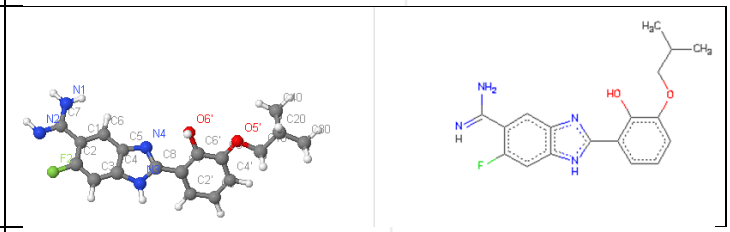
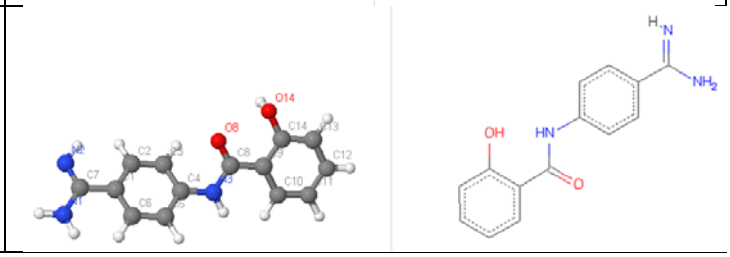
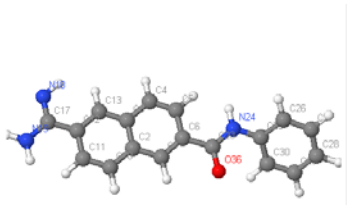
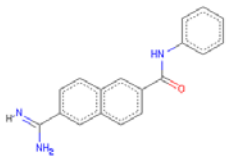
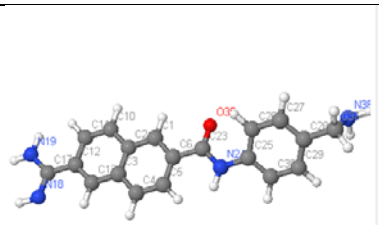
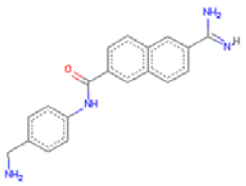
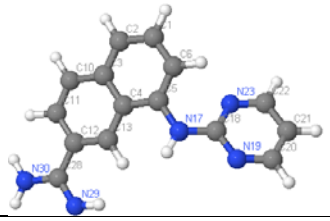
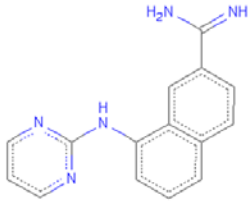
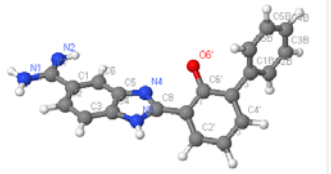
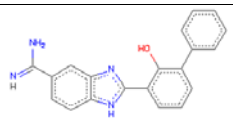
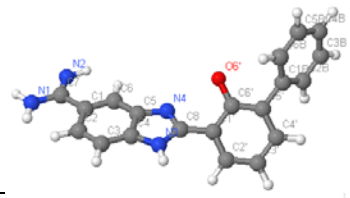
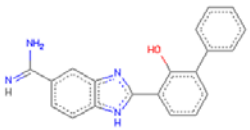
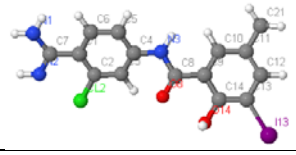
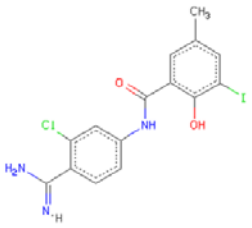
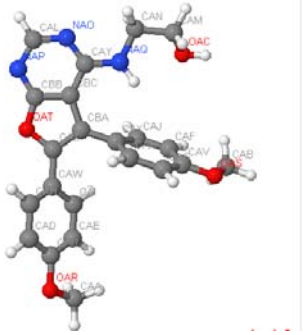
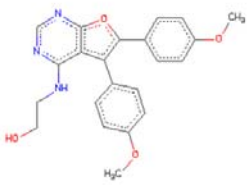
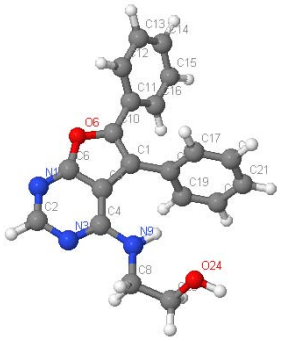
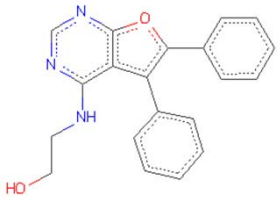
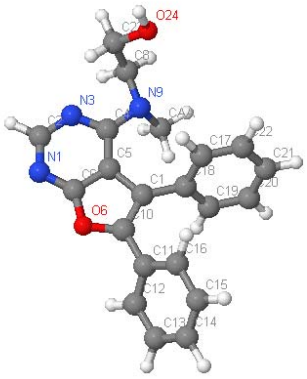
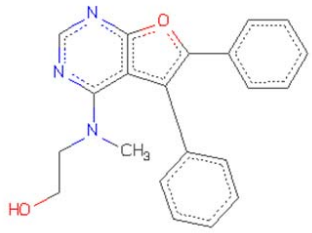
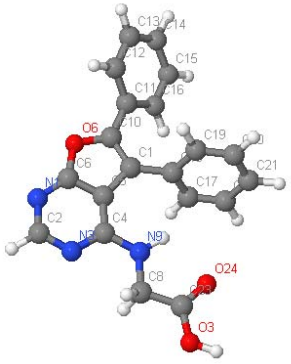
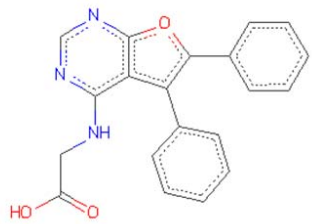
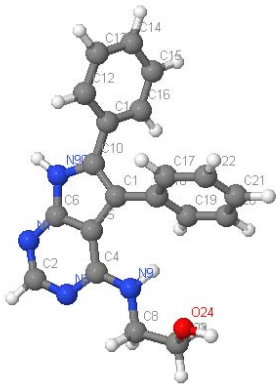
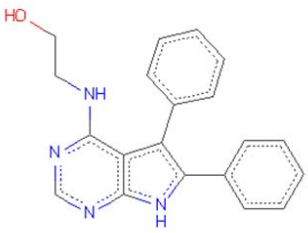
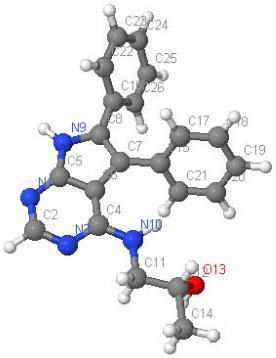
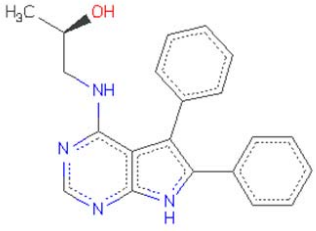
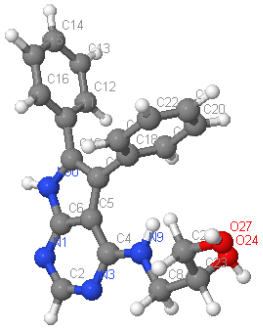
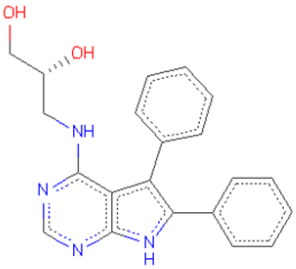
urokinase-type plasminogen activator

1gi7	Ki=31uM	−6. 13	
1gi8	Ki=8.9uM	−6. 86	
1gi9	Ki=6.0uM	−7. 09	
1gj7	Ki=0.013uM	−10. 71	
1gj8	Ki=0.11uM	−9. 45	
1gja	Ki=3.8uM	−7. 36	

1owe	Ki=0.63 uM	−8. 42282	  -
1owh		−10. 05	 
1SQO		−10. 13	 
1gjb	Ki=0.45 uM	−8. 62	 
1gjc	Ki=0.45 uM	−8. 62	 
1gjd	Ki=6.0u M	−7. 09	 

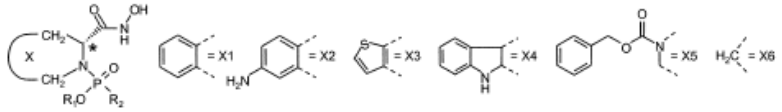
Serine/threonine protein kinase chk1

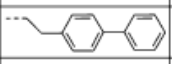
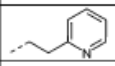
2br1	Ki=7.2uM	−6. 99		
2brb	Ki=13.7uM	−6. 61		
2brg	IC50=6.1uM	−7. 08		

2brh	IC50=22.9uM	-6.30		
2brm	Ki=1.3uM	-8.00		
2brn	IC50=5.5uM	-7.15		
2bro	IC50=1.4uM	-7.95		

MMP-9 (1GKC)

1. Structures, Inhibition Constants,[70] and the Simulation Results of the Studied MMP-9 Inhibitors



No	X	R_1	R_2	log(1/K_i), K_i in M		-Δ<E_{vdw}> [a] (kcal/mol)	-Δ<E_e> [a] (kcal/mol)	-Δ<E_{GBSolv}> [b] (kcal/mol)		-Δ<SASA> (Å^2)	
				Exp.	Calc. [d]			Min.	MD	Min. [c]	MD [a]
1	X1	CH_2CH_3		8.297	8.035	111.93	189.63	1216.74	689.95	417.06	389.34
2 [e]	X1	CH_2CH_3		6.457	6.728	86.41	192.93	1177.15	489.14	324.51	311.53
3	X1	CH_3		8.693	8.819	107.04	174.78	1130.66	860.87	350.53	411.94
4	X1			8.182	7.803	106.40	169.62	1105.70	721.32	425.77	343.59
5	X1			8.341	8.233	95.40	155.90	1140.95	520.52	437.80	496.27
6	X1			8.189	8.315	121.79	192.67	723.49	736.12	370.67	404.37
7	X1	$(CH_2)_2N(CH_2CH_3)_2$		7.777	7.924	72.34	148.89	1107.33	646.02	455.69	395.52
8	X1			8.466	8.337	127.92	239.22	1090.74	533.07	460.21	504.04
9	X1	$(CH_2)_2OCH_2CH_3$		8.197	8.322	120.93	190.55	980.36	746.42	381.41	400.46
10	X1	CH_2CH_3		7.370	7.226	88.32	159.09	874.43	639.75	320.68	305.84
11	X1	CH_2CH_3		7.379	7.562	103.30	179.29	1016.72	696.22	353.45	323.61
12	X1	CH_2CH_3		7.285	7.253	88.67	192.33	879.98	614.65	303.00	321.47
13	X1	CH_2CH_3		7.096	7.017	90.80	182.57	868.42	589.55	316.57	302.09
14	X1	CH_2CH_3		7.493	7.122	98.18	176.21	879.45	595.82	322.45	312.99
15	X1	CH_2CH_3		6.556	7.218	87.85	156.83	887.22	608.37	348.26	319.82
16	X1	CH_2CH_3		7.020	7.635	95.44	183.74	982.55	696.22	334.14	333.28
17	X1	CH_2CH_3		7.228	7.224	94.51	159.36	949.87	595.82	319.49	326.53
18	X1	CH_2CH_3		7.848	8.158	123.38	183.20	1307.85	551.90	459.85	471.31
19	X1	CH_2CH_3		9.509	9.197	121.99	227.93	1127.44	940.95	429.04	423.94
20	X1	CH_2CH_3		10.10	10.18	123.45	206.88	1121.86	834.28	451.32	604.77
21	X1	CH_2CH_3		9.222	8.554	124.01	195.86	1058.55	740.15	456.49	434.23
22	X1	CH_2CH_3		10.00	9.977	137.04	224.55	1127.20	771.52	472.26	608.05
23	X1	CH_2CH_3		7.417	7.675	111.28	197.02	1037.06	771.52	389.28	302.73
24	X2	CH_2CH_3		7.959	8.114	0.74	0.82	1023.59	727.60	384.47	381.87
25	X3	CH_2CH_3		8.420	8.026	103.83	203.22	1013.16	683.67	361.72	391.05
26	X4	CH_2CH_3		8.947	9.193	110.63	189.12	1009.13	771.52	345.50	504.02
27	X5	CH_2CH_3		8.284	8.218	132.48	237.82	879.21	740.15	428.73	389.68
28	X6	CH_2CH_3		6.500	6.081	95.55	180.16	549.68	464.73	253.08	237.38