

Table S1. Known TNKS-1/2 inhibitors for virtual screening method validations.

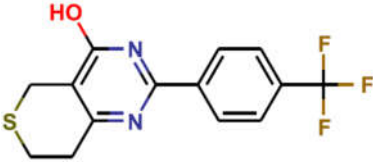
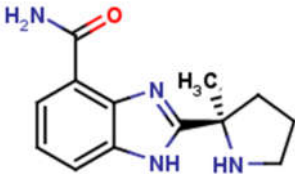
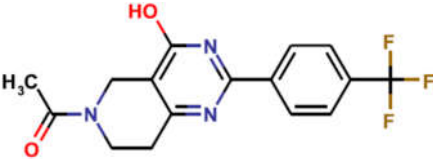
	Compounds	Structur	IC ₅₀ (μM)	
			TNKS-1	TNKS-2
Positive compounds	XAV939		0.011	0.004
	ABT-888		14.97	6.519
Negative compounds	LDW643		>18.75	>18.75

Table S2. The scoring results of training set compounds in each round screening.

	The first screening		The second screening		The third screening
Program	Dock 6.5		Autodock 4.2 (kcal/mol)		
	(kcal/mol)		Rigid docking		Flexible docking
Target	TNKS-1	TNKS-2	TNKS-1	TNKS-2	TNKS-2
XAV939	-23.3976	-48.7548	-7.27	-10.33	-9.15
ABT-888	-13.1766	-14.9015	-6.17	-9.61	-9.10
LDW643	4.0496	72.1593	-5.83	-8.17	-8.25
Selection criteria	Score <-25	Score <-40	Score < -7	Score < -10	Score < -8.5

Table S3. The list of hit compounds by virtual screening (kcal/mol).

No.	ZINC ID	Score	No.	ZINC ID	Score	No.	ZINC ID	Score
1	ZINC52797443	-11.77	2	ZINC49256676	-11.74	3	ZINC50076297	-11.62
4	ZINC48532432	-11.52	5	ZINC46707602	-11.41	6	ZINC49212160	-11.27
7	ZINC08665842	-11.19	8	ZINC49212158	-11.18	9	ZINC41494598	-11.16
10	ZINC41838563	-10.99	11	ZINC06523275	-10.97	12	ZINC00046136	-10.92
13	ZINC40464810	-10.89	14	ZINC48852264	-10.87	15	ZINC00558197	-10.82
16	ZINC30711763	-10.82	17	ZINC48460931	-10.8	18	ZINC04002868	-10.79
19	ZINC22276480	-10.79	20	ZINC02805543	-10.77	21	ZINC15841372	-10.77
22	ZINC04002868	-10.76	23	ZINC47178751	-10.75	24	ZINC08976550	-10.73
25	ZINC03410028	-10.71	26	ZINC14199385	-10.71	27	ZINC41503931	-10.71
28	ZINC17945479	-10.69	29	ZINC41494382	-10.68	30	ZINC21190150	-10.66
31	ZINC24684711	-10.66	32	ZINC40217444	-10.66	33	ZINC13540066	-10.65
34	ZINC00045867	-10.62	35	ZINC17945482	-10.59	36	ZINC46441514	-10.59
37	ZINC46706224	-10.59	38	ZINC41817520	-10.56	39	ZINC51476603	-10.55
40	ZINC16524412	-10.54	41	ZINC20478435	-10.54	42	ZINC00117759	-10.53
43	ZINC01633452	-10.53	44	ZINC19618576	-10.53	45	ZINC05897357	-10.52
46	ZINC41494476	-10.52	47	ZINC45145474	-10.52	48	ZINC48312042	-10.52
49	ZINC20457194	-10.51	50	ZINC19229951	-10.5	51	ZINC46440763	-10.5
52	ZINC08736925	-10.49	53	ZINC41540248	-10.49	54	ZINC46302999	-10.49
55	ZINC48789716	-10.49	56	ZINC05897522	-10.48	57	ZINC46440960	-10.48
58	ZINC19299726	-10.47	59	ZINC20501285	-10.46	60	ZINC41261592	-10.46
61	ZINC07682439	-10.45	62	ZINC29024748	-10.45	63	ZINC00403751	-10.44
64	ZINC13218630	-10.44	65	ZINC08013743	-10.43	66	ZINC36649351	-10.43
67	ZINC52634096	-10.43	68	ZINC18157250	-10.42	69	ZINC18154570	-10.42
70	ZINC48163626	-10.42	71	ZINC06883349	-10.4	72	ZINC48532834	-10.4
73	ZINC18916048	-10.39	74	ZINC23056157	-10.39	75	ZINC24764587	-10.39
76	ZINC06942491	-10.38	77	ZINC31662108	-10.38	78	ZINC36150225	-10.38
79	ZINC06565834	-10.37	80	ZINC47211461	-10.37	81	ZINC42625404	-10.36
82	ZINC00106579	-10.35	83	ZINC16545658	-10.35	84	ZINC04473189	-10.34
85	ZINC06128147	-10.34	86	ZINC05123806	-10.32	87	ZINC18045297	-10.32
88	ZINC44599448	-10.32	89	ZINC48511047	-10.32	90	ZINC01393082	-10.31
91	ZINC03513118	-10.31	92	ZINC03945150	-10.31	93	ZINC06173862	-10.31
94	ZINC06402594	-10.31	95	ZINC12234495	-10.31	96	ZINC35683920	-10.3
97	ZINC06232957	-10.29	98	ZINC29992439	-10.29	99	ZINC31738761	-10.29
100	ZINC32722157	-10.29	101	ZINC39558284	-10.28	102	ZINC44599505	-10.28
103	ZINC49513822	-10.28	104	ZINC06321701	-10.27	105	ZINC18916147	-10.27
106	ZINC32593744	-10.27	107	ZINC40641689	-10.27	108	ZINC46441871	-10.27
109	ZINC00482100	-10.26	110	ZINC12908231	-10.26	111	ZINC41546180	-10.26
112	ZINC24237232	-10.25	113	ZINC46440752	-10.25	114	ZINC52168652	-10.25
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130	ZINC46440554	-10.18	131	ZINC46440582	-10.18	132	ZINC47326869	-10.18
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139	ZINC51508211	-10.16	140	ZINC01582618	-10.15	141	ZINC41545894	-10.15
142	ZINC41546118	-10.15	143	ZINC06484711	-10.15	144	ZINC47326892	-10.15
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223	ZINC45786257	-9.78	224	ZINC41502332	-9.77	225	ZINC04912659	-9.76
226	ZINC25393269	-9.76	227	ZINC48939139	-9.76	228	ZINC05743391	-9.75
229	ZINC48441556	-9.75	230	ZINC16545596	-9.74	231	ZINC42630735	-9.74
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265	ZINC07050319	-9.57	266	ZINC41311355	-9.57	267	ZINC32118579	-9.56
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289	ZINC03403999	-9.48	290	ZINC05090183	-9.48	291	ZINC03231105	-9.47
292	ZINC20535874	-9.47	293	ZINC06218408	-9.46	294	ZINC32119018	-9.46
295	ZINC00652514	-9.45	296	ZINC17178772	-9.45	297	ZINC44078711	-9.45
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304	ZINC05569817	-9.42	305	ZINC06061644	-9.42	306	ZINC47835379	-9.42
307	ZINC00258875	-9.41	308	ZINC07953215	-9.41	309	ZINC07263344	-9.4
310	ZINC09742648	-9.39	311	ZINC41899422	-9.39	312	ZINC36803126	-9.39
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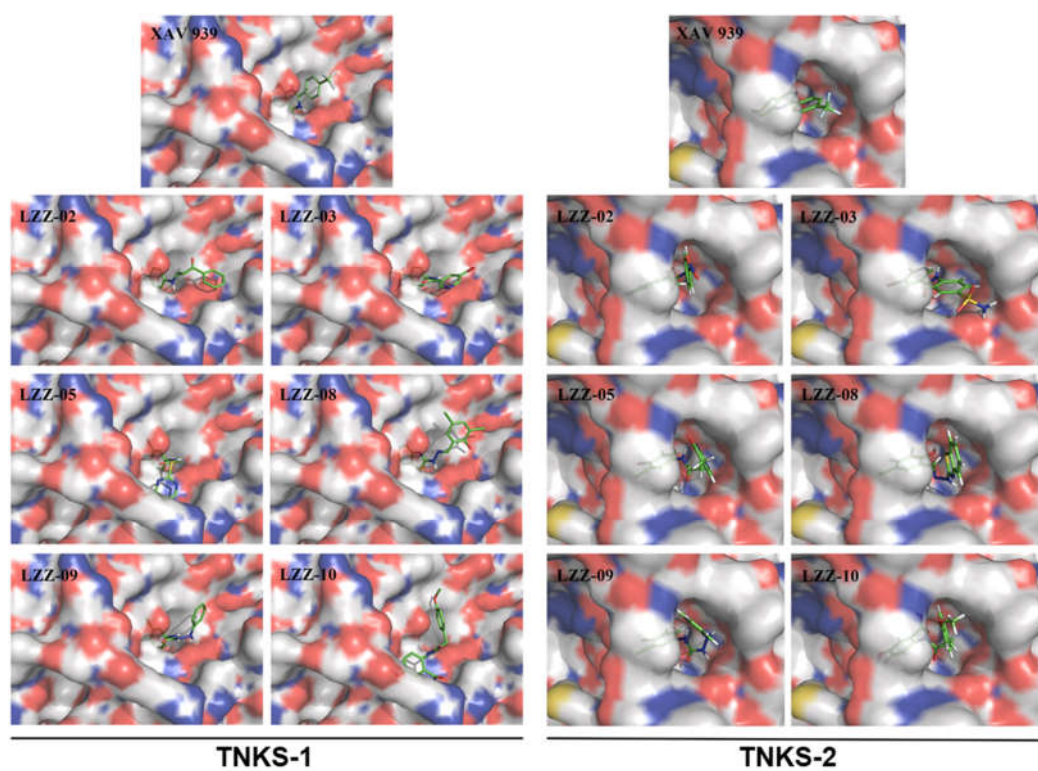


Figure S1. Binding conformation of the selected 6 compounds. XAV939 as the positive control show similar conformation.

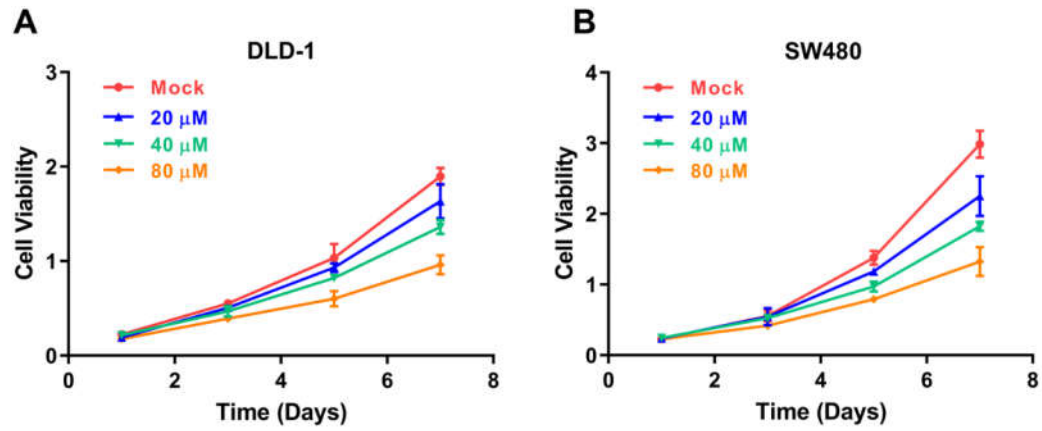


Figure S2. LZZ-02 reduces proliferation in dose-dependent of human colorectal cancer cell.
The DLD-1 (A) and SW480 (B) cell line were treated different concentration of LZZ-02.