

Supplementary table S1: Primers used for the qPCR experiments.

(5'→3')

Actin -F	TTG TTA CAG GAA GTC CCT TGC C
Actin -R	ATG CTA TCA CCT CCC CTG TGT G
AKT1 -F2	CTA CCC ACA CAG CAG TAC GC
AKT1 -R2	AAG TCG CTG GTG TTA AGC CG
CD133 -F	TTC TTG ACC GAC TGA GAC CCA
CD133 -R	TCA TGT TCT CCA ACG CCT CTT
CDK6 -F	CCA GAT GGC TCT AAC CTC AGT
CDK6 -R	AAC TTC CAC GAA AAA GAG GCT T
β-catenin -F	ACT GGC AGC AAC AGT CTT ACC
β-catenin -R	TTT GAA GGC AGT CTG TCG TAA T
STAT3 -F	ACC AGC AGT ATA GCC GCT TC
STAT3 -R	GCC ACA ATC CGG GCA ATC T
mTOR -F	CTG GGA CTC AAA TGT GTG CAG TTC
mTOR -R	GAA CAA TAG GGT GAA TGA TCC GGG
Nanog -F	ATG GAG GAG GGA AGA GGA GA
Nanog -R	GAT TTG TGG GCC TGA AGA AA
SOX2 -F	ACA CCA ATC CCA TCC ACA CT
SOX2 -R	GCA AAC TTC CTG CAA AGC TC

Supplementary table S2: primary antibodies used for western blot analysis.

β -actin	1:5000	Proteintech, Beta Actin Antibody, Rabbit Polyclonal , 20536-1-AP
α -tubulin	1:2000-1:5000	Proteintech, alpha Tubulin Antibody, Rabbit Polyclonal , 11224-1-AP
Akt	1:1000	Cell Signaling, Akt Antibody, Rabbit, #9272
p-Akt	1:1000	Cell Signaling, Phospho-Akt (Ser473) (D9E) XP® Rabbit mAb #4060
CDK6	1:1000	Cell Signaling, CDK6 (DCS83) Mouse mAb, #3136
GAPDH	1:5000-20000	Proteintech, GAPDH Antibody, Rabbit Polyclonal, 10494-1-AP
mTOR	1:1000	Cell Signaling, mTOR (7C10) Rabbit mAb #2983
p-mTOR	1:1000	Cell Signaling, Phospho-mTOR (Ser2481) Antibody #2974
p-mTOR	1:500-1:1000	ABclonal, Phospho-mTOR-S2448, Rabbit mAb, AP0115
NF- κ B	1:1000	Cell Signaling, NF- κ B p65 (D14E12) XP® Rabbit mAb #8242
STAT3	1:1000	Cell Signaling, Stat3 (79D7) Rabbit mAb, #4904
p-STAT3	1:1000	Cell Signaling, Phospho-Stat3 (Tyr705) (D3A7) XP® Rabbit mAb, #9145
STAT3	1:500-1:2000	ABclonal, STAT3, Rabbit pAb, A11216
p-STAT3	1:500-1:2000	ABclonal, Phospho-Stat3-Y708, Rabbit pAb, AP0070
STK4	1:500-1:2000	ABclonal, STK4, Polyclonal Antibody, A8043
TGF- β 1	1:1000	Proteintech, TGF-Beta 1 Antibody, Rabbit Polyclonal, 18978-1-AP
WISP1	1:500-1000	Proteintech, WISP1 Antibody, Rabbit polyclonal , 18166-1-AP
KRAS	1:2000	Proteintech, KRAS Antibody, Rabbit polyclonal, 12063-1-AP
p-Raf 1 (Ser259)	1:1000	EnoGene, Raf-1 (Phospho-Ser259) Rabbit, E011006
p-Mek 1 (Ser221)	1:1000	EnoGene, MEK1 (Phospho-Ser221) Rabbit, E11-7147A
GAPDH	1:5000-10000	Proteintech, GAPDH Antibody, Rabbit Polyclonal, 10494-1-AP

Supplementary table S3: SWISSADME predicted GBM-N019 potential drug target

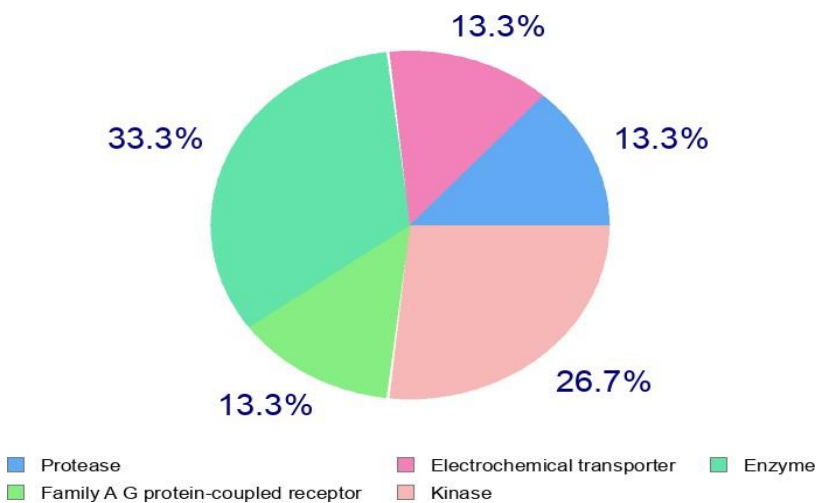
Target	Common Uniprot ID name		ChEMBL ID	Target Class
PI3-kinase p110-delta subunit	PIK3CD	O00329	CHEMBL3130	Enzyme
PI3-kinase p110-beta subunit	PIK3CB	P42338	CHEMBL3145	Enzyme
PI3-kinase p110- gamma subunit	PIK3CG	P48736	CHEMBL3267	Enzyme
Cyclin-dependent kinase 6	CDK6	Q00534	CHEMBL2508	Kinase
Cyclin-dependent kinase 4	CDK4	P11802	CHEMBL331	Kinase
Cyclin-dependent kinase 9	CDK9	P50750	CHEMBL3116	Kinase
Inhibitor of nuclear factor kappa B kinase beta subunit	IKBKB	O14920	CHEMBL1991	Kinase
Inhibitor of NF-kappa- B kinase (IKK)	CHUK	O15111	CHEMBL3476	Kinase
Signal transducer and activator of transcription	STAT	P42226	CHEMBL5401	Transcription factor
Serine/threonine- protein kinase mTOR	MTOR	P42345	CHEMBL2842	Kinase

Supplementary table S4: Drug likeness and ADME property of GBM-N019

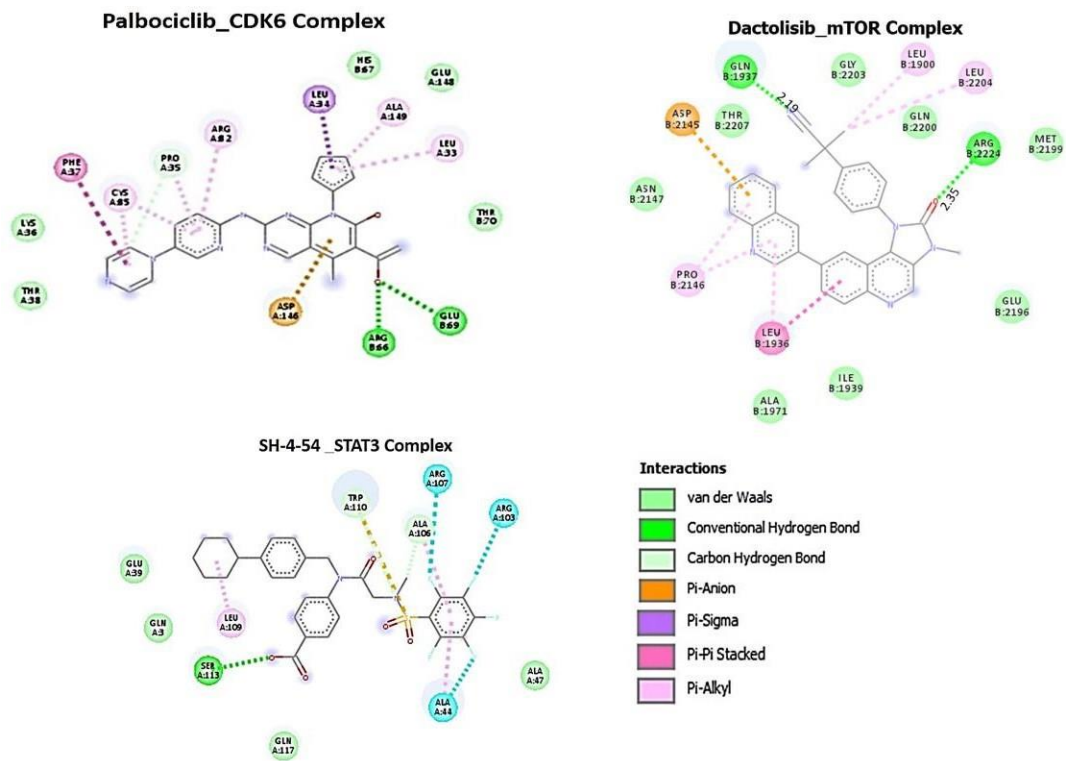
Physicochemical Properties	GBM_N019	Acceptable limit
Molecular Weight	413.92 g/mol	≤ 500
Violation of Lipinski's rule	0	0
No of Rotatable bonds	7	<10
No of H-bond donor	3	≤ 5
No of H-acceptor	4	≤10
Molar refractivity	118.41	40-130
Total polar surface area	102.49 Å ²	≤ 100
Consensus Log Po/w	4.02	≤ 5
Synthetic accessibility	3.26	1(best) - 10(poor)

Supplementary table S5: molecular docking profiles of GBM-0N19 with STAT3, mTOR and CDK6

	NSC77720 5_mTOR	DIS (Å)	NSC777207 _CDK6	DIS (Å)		NSC777207_STAT3
ΔG =(Kcal/mol)	-7.6		-8.1			-6.9
No. hydrophobic contact	4		3			
Conventional H-bond	ASN1899 GLN1937	2.79 3.07	VAL64 VAL77	2.80 2.07		ASN5
C-H bond	PRO1940	3.59	HIS78	3.39		
Halogen bond						GLN66
π -sigma	GLN1937					
π -cation						
π -alkyl	ILE1939 LEU1900		ARG78			
π - π stacked						PHE33 TYR79
Amide- π stacked			GLU72			
Van der waal forces	GLN2200 ALA1971 LEU1939 ASP2145 PRO2146 GLY1897 ASN1898		PRO74 LYS160 PHE135 LEU135 LEU68 VAL76 LEU65 GLU69 LEU79			PHE71 GLN67 ARG70 PRO36 SER2 ALA35 GLN32



Supplementary figure S1. SWISSADME predicted classes of GBM-N019 potential drug target



Supplementary Figure S2: molecular docking profiles of standard inhibitors with STAT3, mTOR and CDK6

Figure 4E

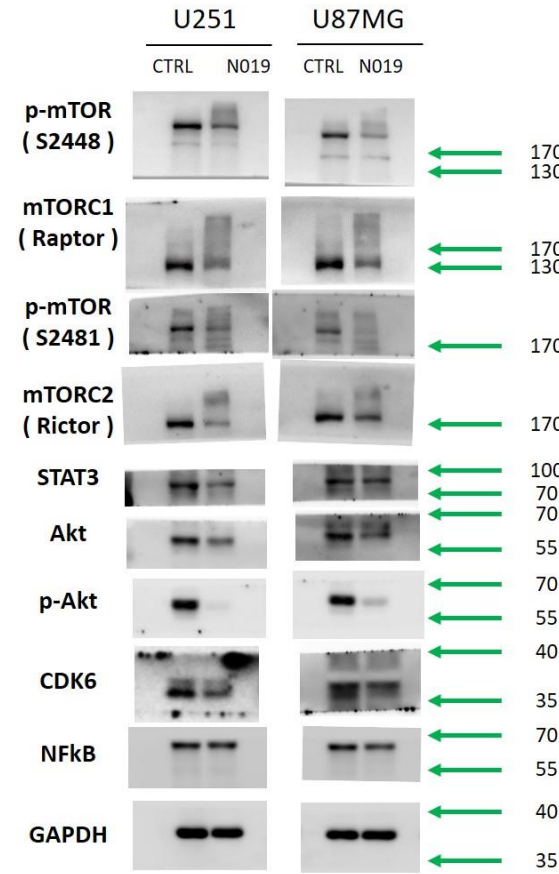


FIGURE 5C

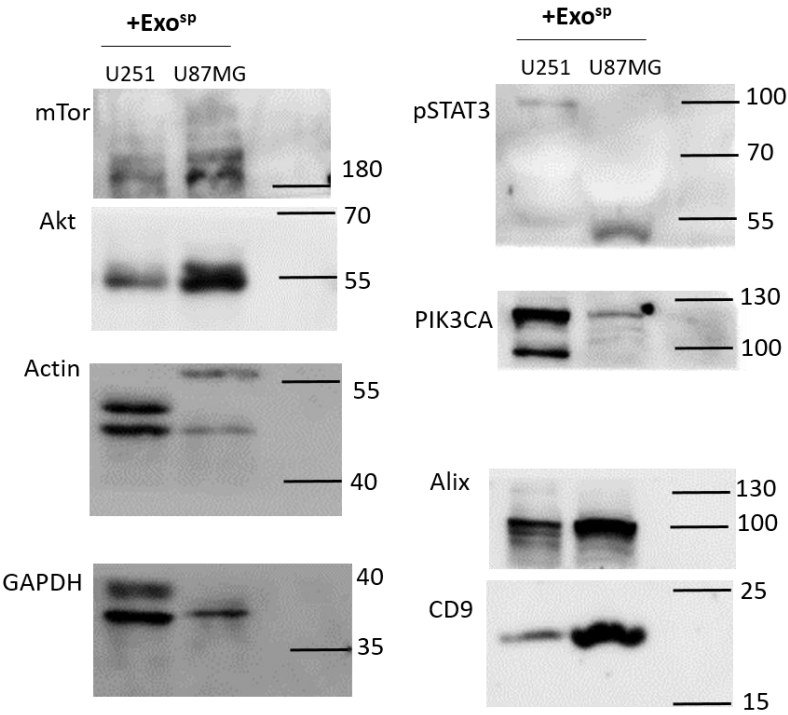


Figure 6D

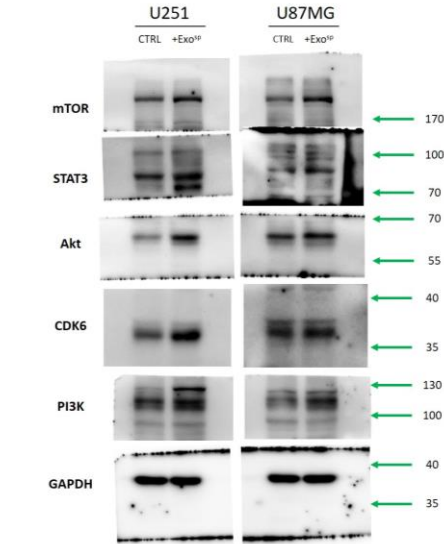


FIGURE 7D

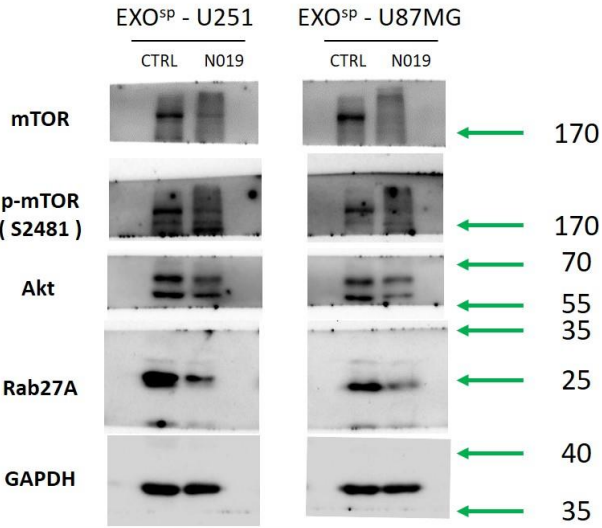


Figure 7. (F)

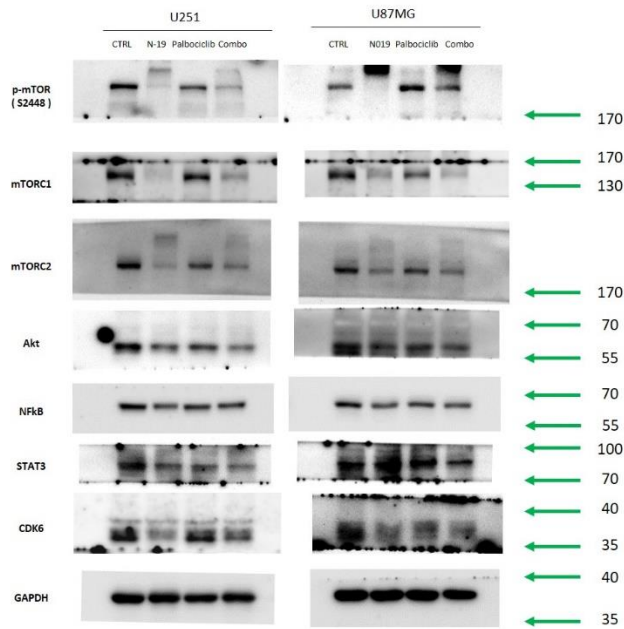
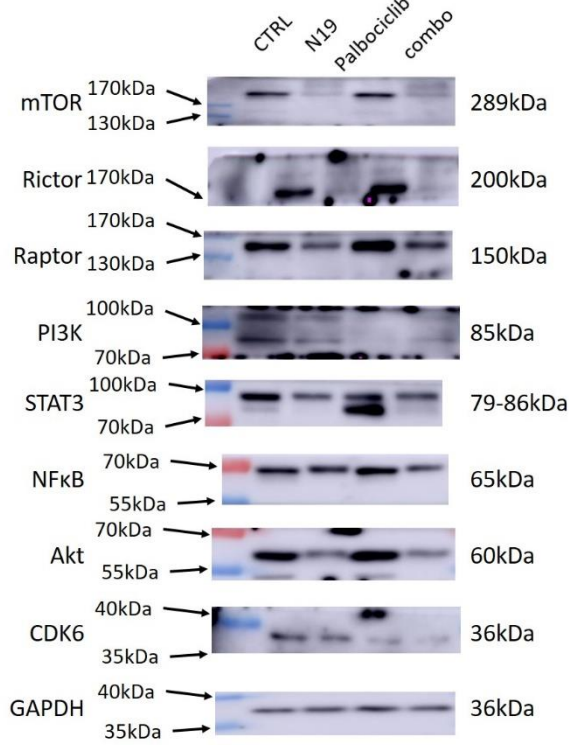


FIGURE 8D



Supplementary Figure S3: Uncropped images of Western blots used in the figures