Supplementary file 1

In silico study of active anticancer peptides from soybean (*Glycine max* (L.) Merr.) as therapeutic agents in hepatocellular carcinoma

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Tabel S1. Predicted Active Site of the Target Protein by PrankWeb

Protein target	Active site residues
SALL4-NuRD	129: B, 131: B, 132: B, 134: B, 183: B, 184: B, 185: B, 187: B, 232: B, 233: B, 234: B, 235: B, 237: B, 279: B, 280: B, 281: B, 283: B, 322: B, 324: B, 325: B, 327: B, 380: B, 381: B, 382: B, 47: B, 48: B, 49: B
VEGF	107: A, 29: A, 31: A, 57: A, 58: A, 59: A, 60: A, 61: A, 66: A, 67: A, 68: A, 31: B, 32: B, 33: B, 34: B, 50: B, 51: B
GPC3	397: A, 398: A, 401: A, 404: A, 405: A, 408: A, 96: A

Tabel S2. Type of Interaction Between the Target Protein and WMLPSYSPY Peptide

Peptide - Protein target	Interactions with SALL4-NuRD residues	
	Hydrogen bond	Hydrophobic interaction
WMLPSYSPY - SALL4-NuRD (-237.813)	Trp 1 : Ser 164 ⇒ 2.90 Å Trp 1 : Gln 166 ⇒ 3.19 Å Trp 1 : Asp 162 ⇒ 2.90 Å	Ser 164 (A) : Met 2 Ser 164 (A): Trp 1 Asn 168 (A): Trp 1 Glu 166 (A): Trp 1 Glu 166 (A): Met 2 Glu 166 (A) : Pro 4

	Tyr 6 : Gln 324 ⇒ 2.21 Å Tyr 6 : Ser 280 ⇒ 2.47 Å Pro 8 : Gln 48 ⇒ 2.95 Å Tyr 9 : Leu 183 ⇒ 2.05 Å Tyr 9 : Leu 183 ⇒ 2.29 Å Tyr 9 : Arg 129 ⇒ 3.31 Å	Asp 162 (A) : Trp 1 Asp 162 (A) : Met 2 Leu 238 (B) : Met 2 Leu 238 (B) : Leu 3 Asn 188 (B) : Met 2 Asn 188 (B) : Pro 4 Pro 187 (B) : Pro 4 Leu 237 (B) : Pro 4 Leu 237 (B) : Tyr 6 Gln 324 (B) : Tyr 6 Gln 324 (B) : Tyr 9 Phe 281 (B) : Tyr 6 Ser 280 (B) : Tyr 6 Leu 183 (B) : Tyr 9 Arg 129 (B) : Tyr 9 Arg 131 (B) : Tyr 9 Gln 48 (B) : Tyr 9 Gln 48 (B) : Pro 8 Trp 325 (B) : Tyr 6 Trp 382 (B) : Pro 8 Pro 384 (B) : Ser 7 Ser 381 (B) : Pro 8 Pro 327 (B) : Ser 7 Pro 283 (B) : Ser 5 Pro 283 (B) : Tyr 6 Pro 283 (B) : Ser 7
WMLPSYSPY - VEGF (-216.15)	Ser 5 : Gly 59 ⇒ 2.81 Å Tyr 6 : Gly 59 : 2.76 Å Tyr 6 : Thr 31 ⇒ 3.31 Å Tyr 9 : Gln 37 ⇒ 2.77 Å	Gln 37 (A) : Tyr 9 Val 33 (A) : Tyr 9 Cys 57 (A) : Pro 8 Arg 56 (A) : Tyr 9 His 99 (A) : Tyr 9 Cys 68 (A) : Tyr 9 Pro 70 (A) : Tyr 9 Val 69 (A) : Tyr 9 Ile 29 (A) : Tyr 6 Leu 32 (B) : Tyr 6 Cys 51 (B) : Ser 5 Cys 51 (B) : Ser 7 Thr 31 (A) : Tyr 6 Thr 31 (A) : Pro 8

		Thr 31 (B) : Tyr 6 Glu 30 (A) : Tyr 6 Asp 34 (B) : Trp 1 Asp 34 (B) : Ser 5 Gln 37 (B) : Trp 1 Phe 36 (B) : Trp 1 Phe 36 (B) : Met 2 Asp 63 (A) : Leu 3 Leu 66 (A) : Leu 3 Glu 64 (A) : Leu 3 Val 33 (B) : Ser 5 Lys 107 (A) : Pro 4 Gly 58 (A) : Tyr 6 Gly 59 (A) : Tyr 6 Gly 59 (A) : Ser 5
WMLPSYSPY - GPC3 (-190.267)	Ser 5 : Tyr 488 ⇒ 2.25 Å	His 412 (A) : Tyr 6 His 412 (A) : Ser 7 His 412 (A) : Pro 8 Leu 92 (A) : Tyr 6 Tyr 408 (A) : Tyr 6 Tyr 408 (A) : Ser 5 Ser 95 (A) : Tyr 6 Ser 95 (A) : Ser 5 Phe 401 (A) : Trp 1 Ala 96 (A) : Trp 1 Ala 96 (A) : Met 2 Phe 398 (A) : Met 2 Glu 99 (A) : Leu 3