

Supplementary material:

Table 1: List of amino acid residues involved in protein-protein interaction between E6-p53 & E7-RB1 as predicted by SHARP2.

Ligand	Receptor	Moldock score	No: of Hbond	Hbond Energy	Amino acids with which Hydrogen Bonds are formed
Nicandrenone	1AD6/RB1	-95.0387	5	-9.38092	Val531, Ser534, Ser463, Val531
	1VZN/E6	-121.578	5	-11.77	Lys79, Tyr99, Glu120, Glu 97
	2B9D/E7	-84.8187	6	-8.13861	Glu74, Asn82, Leu77, val49, glu56
	1TUP/P53	-106.56	5	-8.71093	Thr231, Thr230, Glu221 Glu224 Arg202
Ginsenosides	1AD6/RB1	-99.66408	3	-5.63265	Met460, Lys530, Asp479
	1VZN/E6	-97.1809	3	-3.01999	Glu74
	2B9D/E7	-76.9515	3	-6.97368	Ser51
	1TUP/P53	-96.8829	5	-6.7669	Val97, Asn200, Arg202
Pregnane	1AD6/RB1	-93.7979	0	0	
	1VZN/E6	-120.998	0	0	
	2B9D/E7	-67.0394	0	0	
	1TUP/P53	-89.6934	0	0	
Steriol Glycosides	1AD6/RB1	-89.2408	1	-2.01832	
	1VZN/E6	-119.959	2	3.28452	Ser534
Glycosides	2B9D/E7	-72.9879	2	-1.4832	Glu48
	1TUP/P53	-94.4142	1	-0.847297	Arg71, Ser68

Table 2: Docking Analysis of the four best compounds from the list of 88 compounds screened. Table depicts the Moldock scores, Hydrogen bond interaction and the list of amino acids with which hydrogen bonds are formed.

	E6	P53
Site of interaction of P53-E6	22 LEU , 23 CYS , 41 LYS , 42 GLN , 43 GLN , 45 LEU , 46 ARG , 47 ARG , 49 VAL , 50 TYR , 51 ASP , 53 ALA , 54 PHE , 57 LEU , 71 ASP , 74 LEU , 75 LYS , 76 PHE , 78 SER , 79 LYS 80 ILE , 82 GLU , 83 TYR , 84 ARG 85 HIS , 86 TYR , 99 TYR	110 ARG , 111 LEU , 112 GLY , 113 PHE , 114 LEU , 115 HIS , 116 SER , 124 CYS , 126 TYR , 128 PRO , 131 ASN , 142 PRO , 144 GLN , 146 TRP , 229 CYS , 231 THR
	E7	Rb1
	45 PRO , 46 TYR , 47 ALA , 57 LYS , 58 LEU , 59 VAL , 60 ARG , 61 LEU , 62 THR , 63 VAL , 64 LEU , 73 LEU , 74 GLU , 76 MET , 77 LEU , 81 LEU , 82 ASN , 83 ILE , 84 VAL , 86 PRO , 87 LEU , 89 THR , 90 LEU , 91 GLN 92 ARG , 93 GLN	378 VAL , 379 MET , 380 ASN 381 THR , 382 ILE , 383 GLN 384 GLN , 387 MET , 388 ILE 390 ASN , 497 THR , 498 TYR 499 SER , 500 ARG , 501 SER 503 SER , 531 VAL
	Site of interaction of E7-RB1	