Supplementary Table 1. Interaction Energy Values Calculated on a per residue basis for peptide-cyclin complexes

	Cyclin A		**Cyclin A**		**Cyclin A**		**Cyclin A**		**Cyclin A**
H	-65.1	S	-63.9	P	-23.1				
A	-18.0	A	-19.2	V	-15.8				
K	-42.2	K	-40.6	K	-47.4				
R	-72.3	R	-69.7	R	-74.3	R	-111.3	Cit	-38.4
R	-58.7	R	-25.2	R	-9.3	R	-46.4	R	-47.2
L	-11.7	L	-12.8	L	-9.9	L	-13.8	L	-13.8
I	-6.8	F	-12.2	D	0.6	I	-0.1	I	-0.06
F	-23.5	G	-4.2	L	-15.4	F	-19.5	F	-19.6
total	-298.3		-247.8		-194.6		-191.1		-119.06
	Cyclin D		**Cyclin D**		**Cyclin D**		**Cyclin D**		**Cyclin D**
H	-20	S	-24.1	P	-18.8				
A	-6.3	A	-5.6	V	-11.9				
K	-44.6	K	-44.7	K	-52.2				
R	-54.7	R	-57	R	-47.6	R	-106.9	Cit	-30.3
R	-27	R	-17.6	R	-11.1	R	-19.2	R	-19.2
L	-15.2	L	-13.7	L	-14.7	L	-14.1	L	-14.1
I	0.7	F	-10.2	D	-1.6	I	0.2	I	0.2
F	-13	G	-4.7	L	-11.7	F	-13.9	F	-13.9
TOTAL	-180.1		-177.6		-169.6		-153.9		-77.3

Supplementary Table 2. Binding Energy and Desolvation penlty calculated on peptide-cyclin complexes

Cyclin A	Complex Desolvation Penalty	**Cyclin D**	Complex Desolvation Penalty
SAKRRLFG	3.12	SAKRRLFG	3.23
HAKRRLIF	3.48	HAKRRLIF	3.42
PVKRRLDL	2.93	PVKRRLDL	3.08
RRLIF	2.36	RRLIF	2.47
CitRLIF	2.32	CitRLIF	2.44

1OKV	**CYCLIN A**
HAKRRLIF	cyclin fixed
MET210	-4.7
ILE213	-6.5
LEU214	-3.3
ASP216	-16.7
TRP217	-8.8
GLU220	-28.9
VAL221	-1.6
GLU224	-41.2
ARG250	-9.1
LEU253	-1.4
GLN254	-13
TYR280	-2
ILE281	-3
THR282	-4.9
ASP283	-36.1
THR285	-2.3
TOTAL	-183.5

2W96	**CYCLIN D**
HAKRRLIF	BB FIXED
MET56	-3.8
ILE59	-8.7
VAL60	-2.7
THR62	0.6
TRP63	-6.2
GLU66	-47.4
VAL67	-1.1
GLU70	-18.8
LYS96	-0.9
SER97	-1.2
LEU99	-1.7
GLN100	-8.7
ILE126	-5.2
TYR127	-8.3
THR128	-5.3
ASP129	-50.3
SER131	-6
total	-90.2

Supplementary Table 2. Binding Energetic Data for P27/Cyclin complexes

	cyclin D 2w96	cyclin A 1JSU
Residue	Interaction Energy (kcal/mol)	Interaction Energy (kcal/mol)
C_LYS25	-41.2	-59.4
C_PRO26	-5.4	-3.4
C_SER27	0.3	3.6
C_ALA28	-10.0	-15.0
C_CYS29	-4.1	-7.0
C_ARG30	-44.3	-54.7
C_ASN31	-11.9	-3.0
C_LEU32	-14.1	-14.6
C_PHE33	-15.5	-15.0
C_GLY34	1.8	0.7
C_PRO35	-3.0	-2.7
C_VAL36	-1.9	-3.6
C_ASP37	-3.9	-3.3
C_HIS38	-7.8	10.8
C_GLU39	-0.9	-4.7
C_GLU40	-10.6	-4.1
C_LEU41	-9.1	-3.2
C_THR42	-1.4	-4.2
C_ARG43	-2.8	8.8
C_ASP44	-34.7	-22.9
C_LEU45	-9.8	-8.7
C_GLU46	0.5	19.5
C_LYS47	0.6	5.9
C_HIS48	-1.2	-9.3
C_CYS49	-4.0	-3.7

Name	Forcefield	Total Interaction Energy (kcal/mol)	Total VDW Interaction Energy (kcal/mol)	Total Electrostatic Interaction Energy (kcal/mol)
2W96	CHARMm	-234.52912	-89.36208	-145.16704
1JSU	CHARMm	-193.08529	-51.41365	-141.67164

Supplementary Table 4. Analytical Data for Cyclin A2 and D1 Binding Peptides

Peptide	Purity	Column Dimensions	Method	FlowRate	Retention Time	Theoretical MW	Observed MW
CitRLIF	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	21.8	704.43	704.5
HAKCitRLIF	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	15.1	1041.28	1041.3
HAKRRLIF	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	14.8	1040.27	1040.3
HAKRRLIX1	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	31.9	1029.24	1029.59
HAKRRLIX2	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	21.2	1045.31	1045
HAKRRLIX3	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min		1045.31	1045
HAKRRLIX4	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	15.2	1018.28	1018.2
HAKRRLIX5	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	16.6	1032.31	1031.7
HAKRRLIX6	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	23.3	1045.33	1045
HAKRRLIX7	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	17.4	1040.27	1040.64
HAKTRLIF	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	15.8	985.19	984.6
PAKRRLFG	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	14.1	944.14	943.65
PVKRRL3CFG	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	15.2	1006.7	1005.7
PVKRRLFG	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	13.8	972.19	971.6
RRLIpfF	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	21.8	704.86	704.437
SAKRALFGM	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	16.5	980.19	980.1
SAKRNLFG	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	13.9	891.03	890.5
SAKRNLFGM	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	16.0	1023.22	1023.2
SAKRRLPBA	>90%	4.6 × 250 nm	0-100% acetonitrile/water/0.1%TFA	1ml/min	28.8	911.1	908.6
SAKRRLX1G	>90%	4.6 × 250 nm	12-42% acetonitrile/water/0.1%TFA	1ml/min	10.1	922.9	923.4
SAKRRLX2G	>90%	4.6 × 250 nm	13-43% acetonitrile/water/0.1%TFA	1ml/min	10.3	938.9	939.7
SAKRRLX3G	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	13.3	939.16	939
SAKRRLX4G	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	13.7	911.12	910.6
SAKRRLX5G	>90%	4.6 × 250 nm	5-65% acetonitrile/water/0.1%TFA	1ml/min	14.3	925.15	924.8
SAKRRLX6G	>90%	4.6 × 250 nm	17-47% acetonitrile/water/0.1%TFA	1ml/min	11.2	939.9	940.8
SAKRRLX7G	>90%	4.6 × 250 nm	6-36% acetonitrile/water/0.1%TFA	1ml/min	11.1	934.9	935.8
SAKRRLX8G	>90%	4.6 × 250 nm	10-35% acetonitrile/water/0.1%TFA	1ml/min	9.7	934.06	935.55
SCCP10	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	32.2	721.27	721.2
SCCP5624	>90%	4.6 × 250 nm	0-60% acetonitrile/water/0.1%TFA	1ml/min	26.5	638.8	639

Supplementary Figure 1 (Correlation between IC50 and interaction energy for cyclin A -peptide complexes

Cyclin A	Interaction Energy (Kcal/Mol)	IC50 (µM)	LogIC50
HAKRRLIF	-298.3	0.021	-1.68
SAKRRLFG	-247.8	0.073	-1.14
PVKRRLDL	-194.6	1.2	0.08
RRLIF	-191.1	7.7	0.89