Supporting information

PAMAM/5-flurouracil drug conjugate for targeting E6 and E7 oncoproteins in cervical cancer: a combined experimental/in silico approach†

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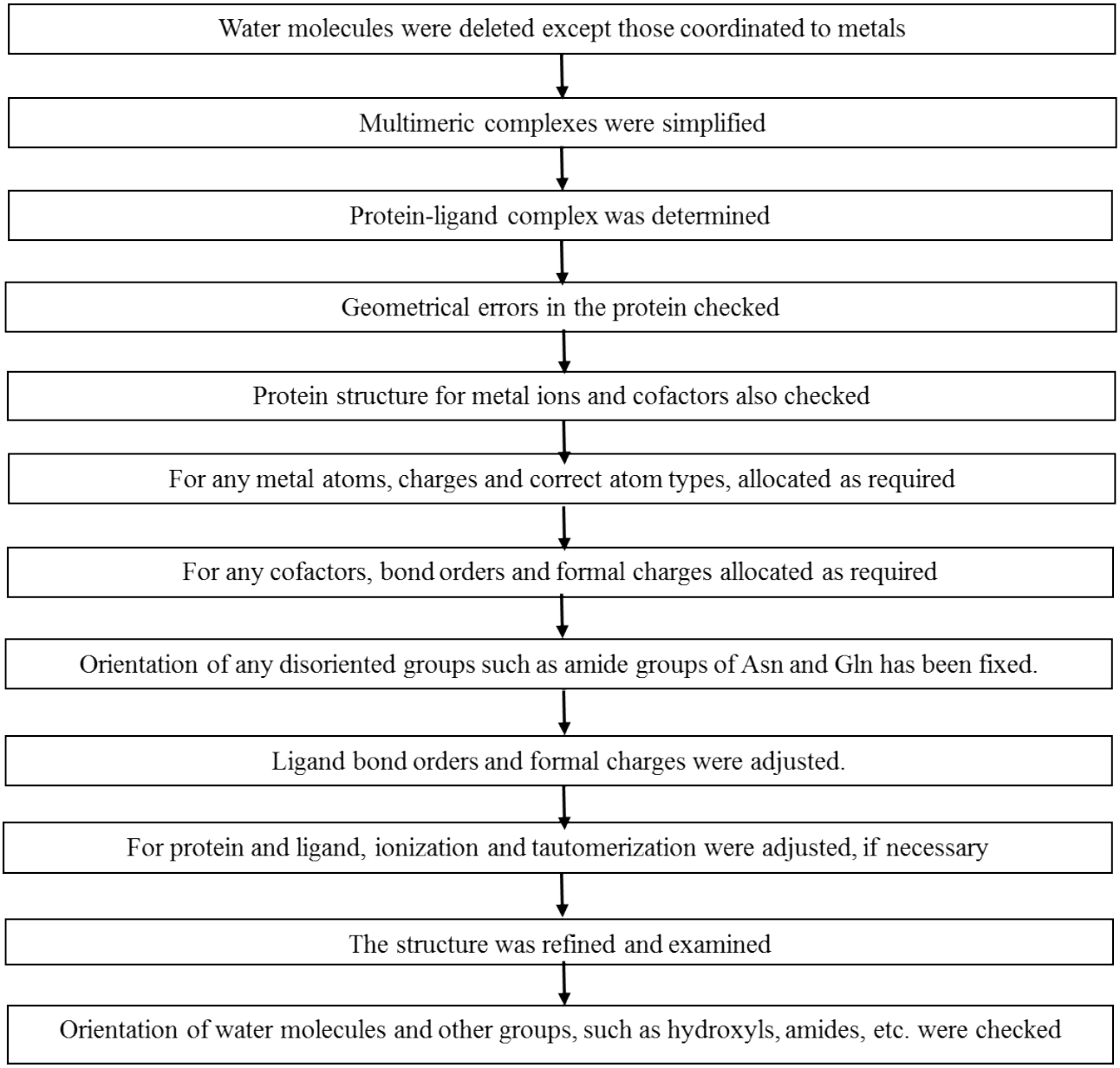
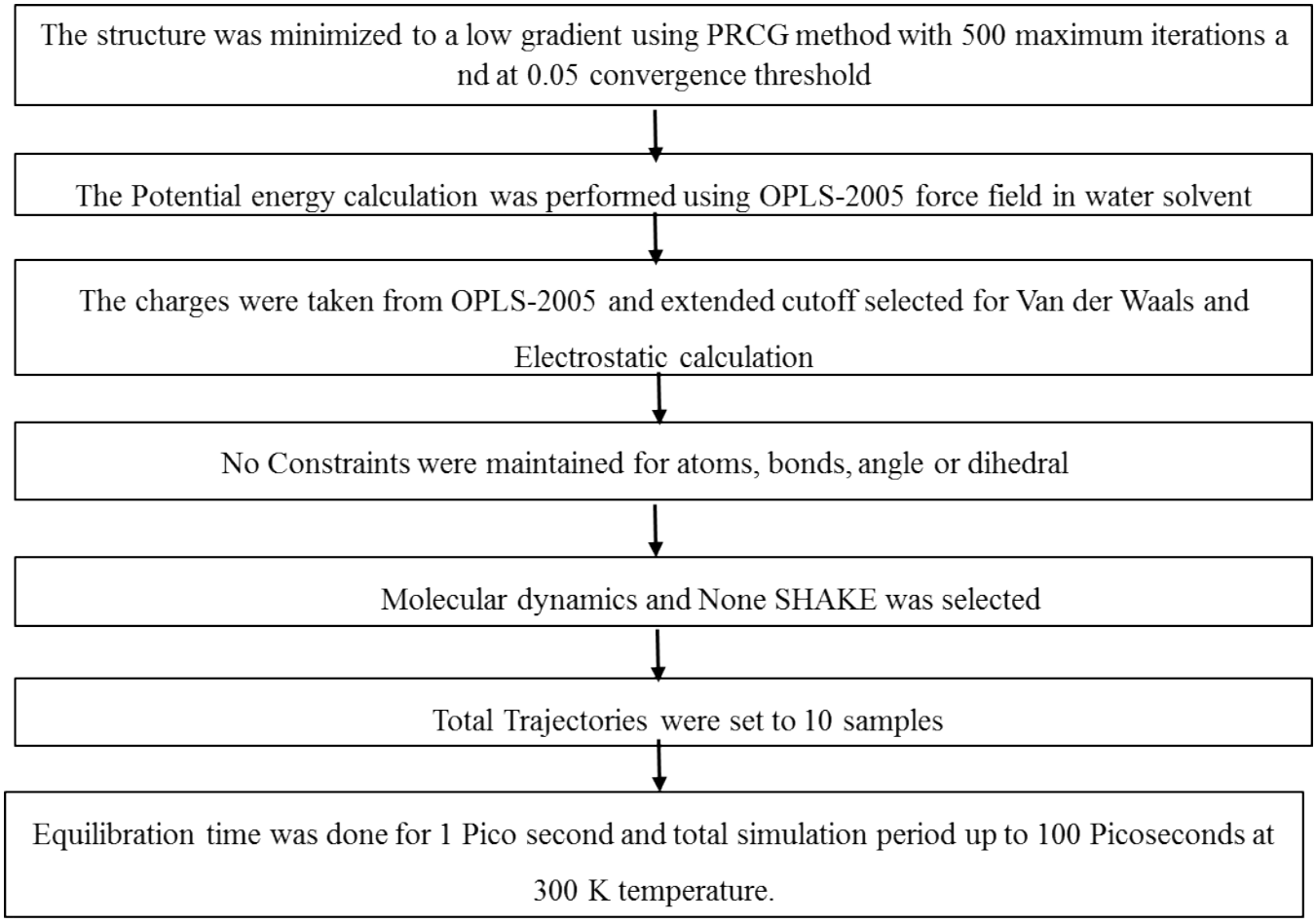
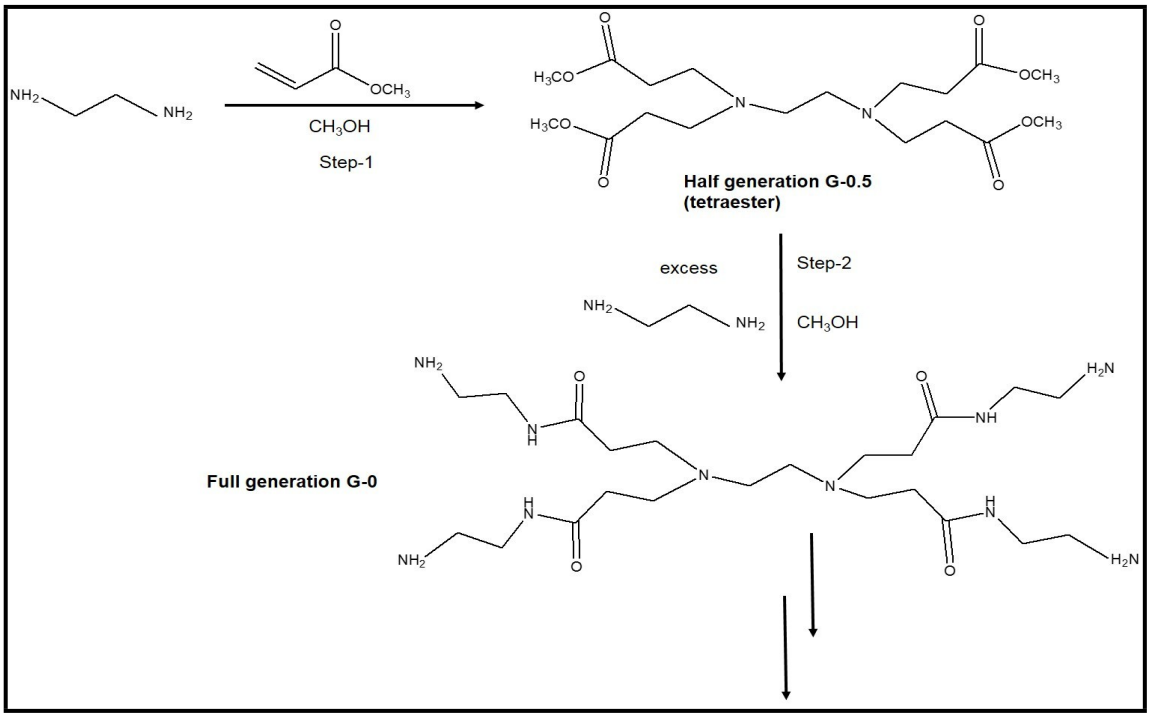


Protocol 1. Protein preparation- Schrödinger suite.



Protocol 2. Methodology and parameters for molecular simulation of E6 and E7 oncoproteins and oncoprotein-5-FU complex.



Scheme S1. Diagram of the synthesis of EDA-core PAMAM dendrimers.

Table S1. Synthesis of different generations of PAMAM using EDA and methyl acrylate

S. No	Dendrimer generations	0.01M PAMAM dendrimer	
		Ethylene diamine (mL)	Methyl Acrylate (mL)
1	0.5G	0.67	7.21
2	1.0G	5.36	-
3	1.5G	-	14.42
4	2.0G	10.71	-
5	2.5G	-	28.85

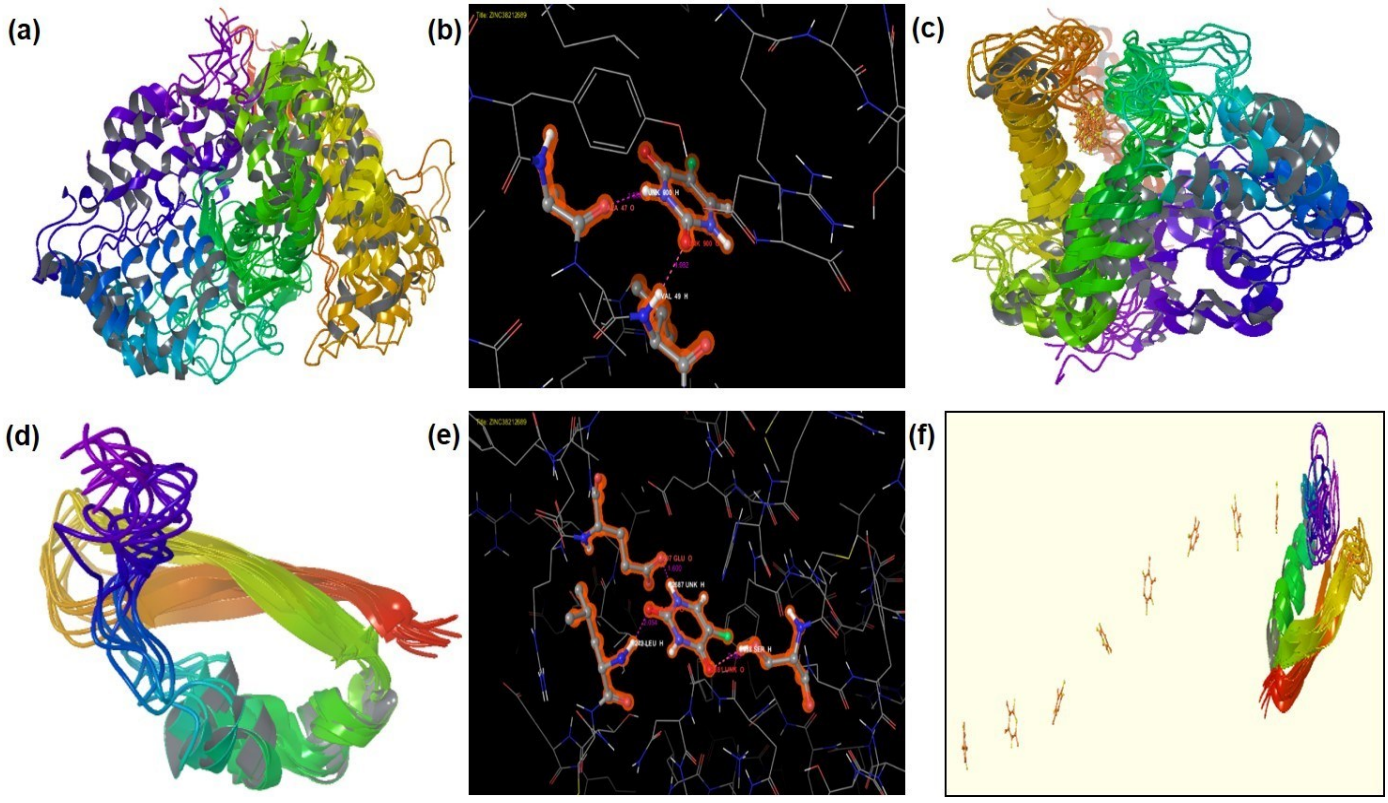


Fig. S1. Molecular docking analysis. (a, d) conformational structure (b, e) interaction profile, and (c, f) RMSD plot of E6 and E7 protein over 5-FU.

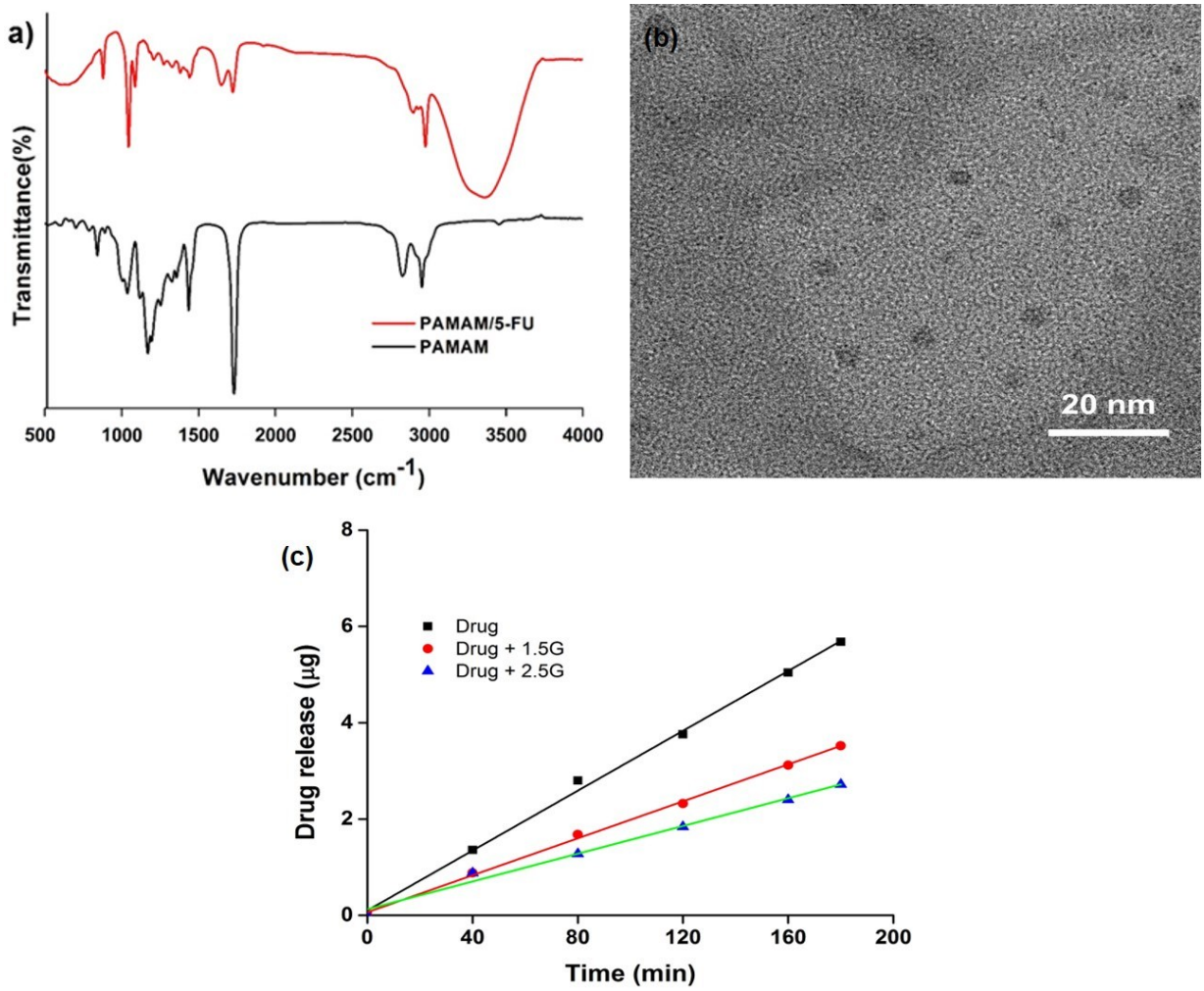


Fig. S2 (a) FTIR spectrum and (b) TEM image of the PAMAM/5-FU complex and (d) Amount of Drug release at different time interval.

Table S2. FTIR bands of PAMAM and PAMAM/5-FU and their corresponding stretching vibrations

S. No	1.5G PAMAM	1.5G PAMAM/5-FU	Spectral assignment
1	3451 cm^{-1}	3366 cm^{-1}	NH stretching
2	2954 cm^{-1}	2972 cm^{-1}	CH_2 Asymmetric stretching
3	2827 cm^{-1}	2891 cm^{-1}	CH_2 Symmetric stretching
4	1645 cm^{-1}	1643 cm^{-1}	C=O stretching
5	1257 cm^{-1}	1275 cm^{-1}	C-N stretching
6	1437 cm^{-1}	1442 cm^{-1}	CH_2 bending
7	-	1088 cm^{-1}	C-F stretching

Table S3. Dynamic light scattering analysis of PAMAM and PAMAM/5-FU

S. No	Sample	PAMAM (nm)	PAMAM/5-FU width (nm)
1	1.5G (0.01M)	2.3	4.2
2	2.5G (0.01M)	5.6	6.9

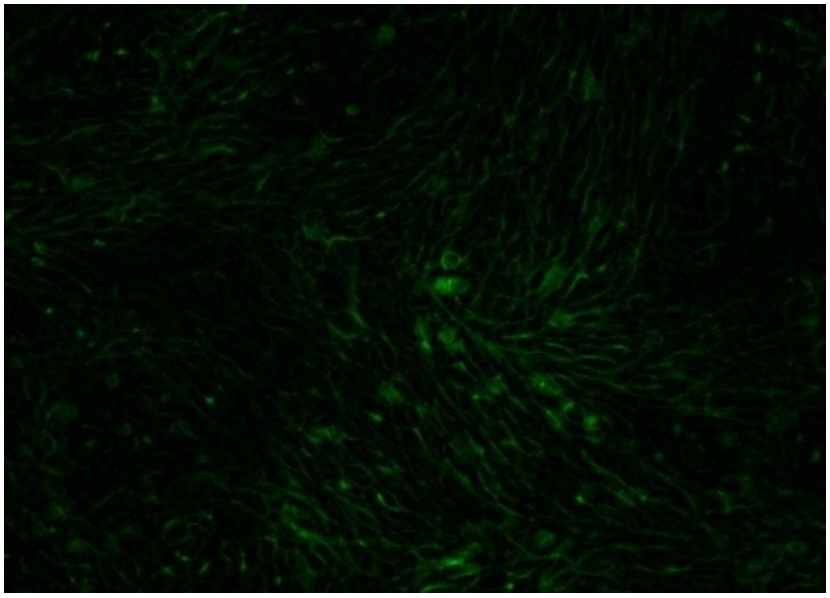
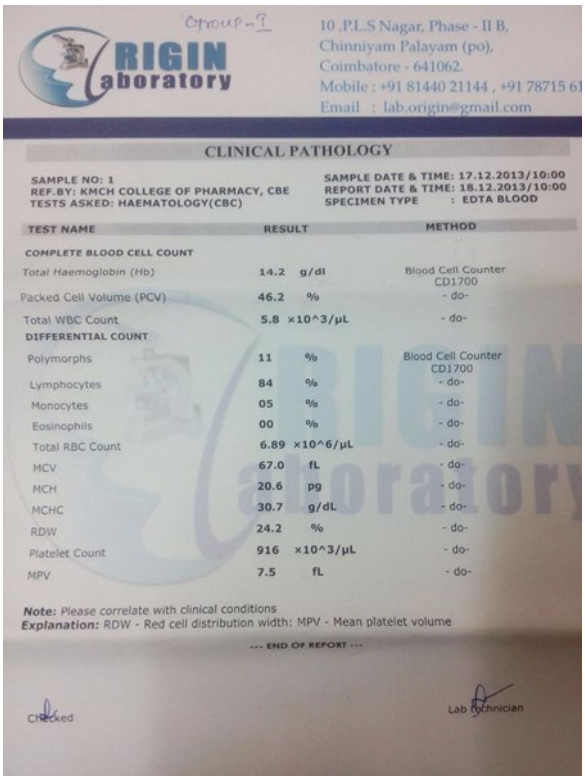


Fig. S3. FITC-Drug conjugate.



Group - I

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CLINICAL PATHOLOGY

SAMPLE NO: 1
REF.BY: KMCH COLLEGE OF PHARMACY, CBE
TESTS ASKED: HAEMATOLOGY(CBC)

SAMPLE DATE & TIME: 17.12.2013/10:00
REPORT DATE & TIME: 18.12.2013/10:00
SPECIMEN TYPE : EDTA BLOOD

TEST NAME	RESULT		METHOD
COMPLETE BLOOD CELL COUNT			
Total Haemoglobin (Hb)	14.2	g/dl	Blood Cell Counter CD1700
Packed Cell Volume (PCV)	46.2	%	- do-
Total WBC Count	5.8	×10^3/µL	- do-
DIFFERENTIAL COUNT			
Polymorphs	11	%	Blood Cell Counter CD1700
Lymphocytes	84	%	- do-
Monocytes	05	%	- do-
Eosinophils	00	%	- do-
Total RBC Count	6.89	×10^6/µL	- do-
MCV	67.0	fL	- do-
MCH	20.6	pg	- do-
MCHC	30.7	g/dL	- do-
RDW	24.2	%	- do-
Platelet Count	916	×10^3/µL	- do-
MPV	7.5	fL	- do-

Note: Please correlate with clinical conditions
Explanation: RDW - Red cell distribution width: MPV - Mean platelet volume

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Checked

Lab Technician

Fig. S4. Hematological analysis of Group-I BALB/c female mice with cervical cancer model.