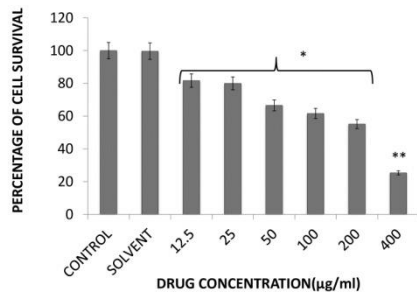
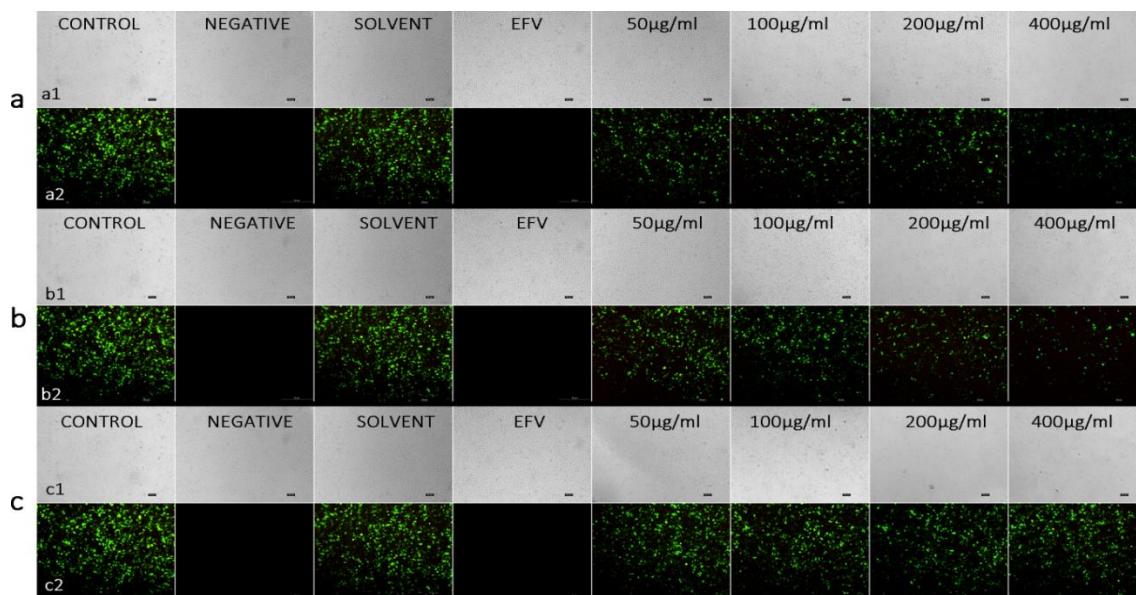


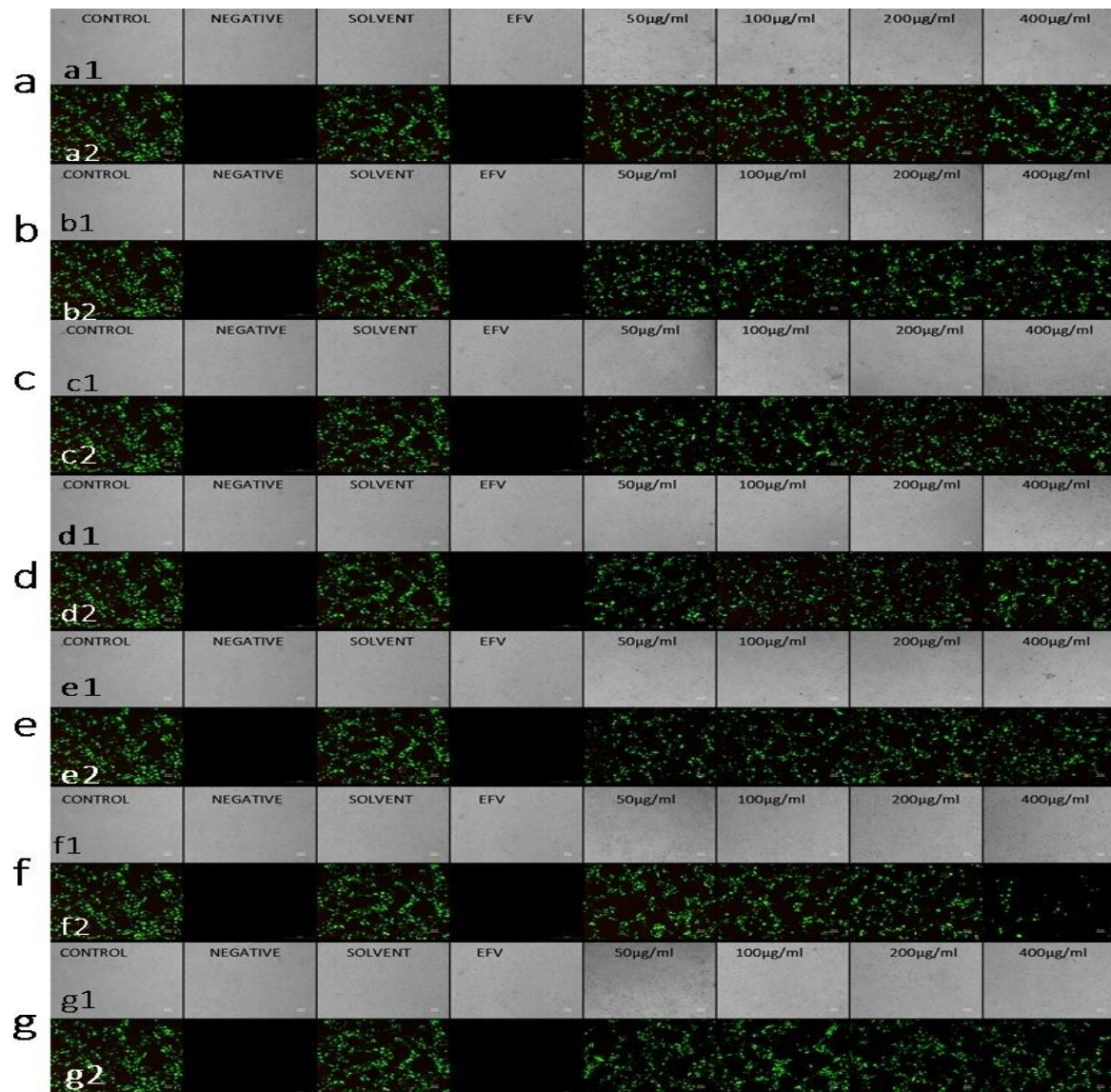
SUPPLEMENTARY FIGURE



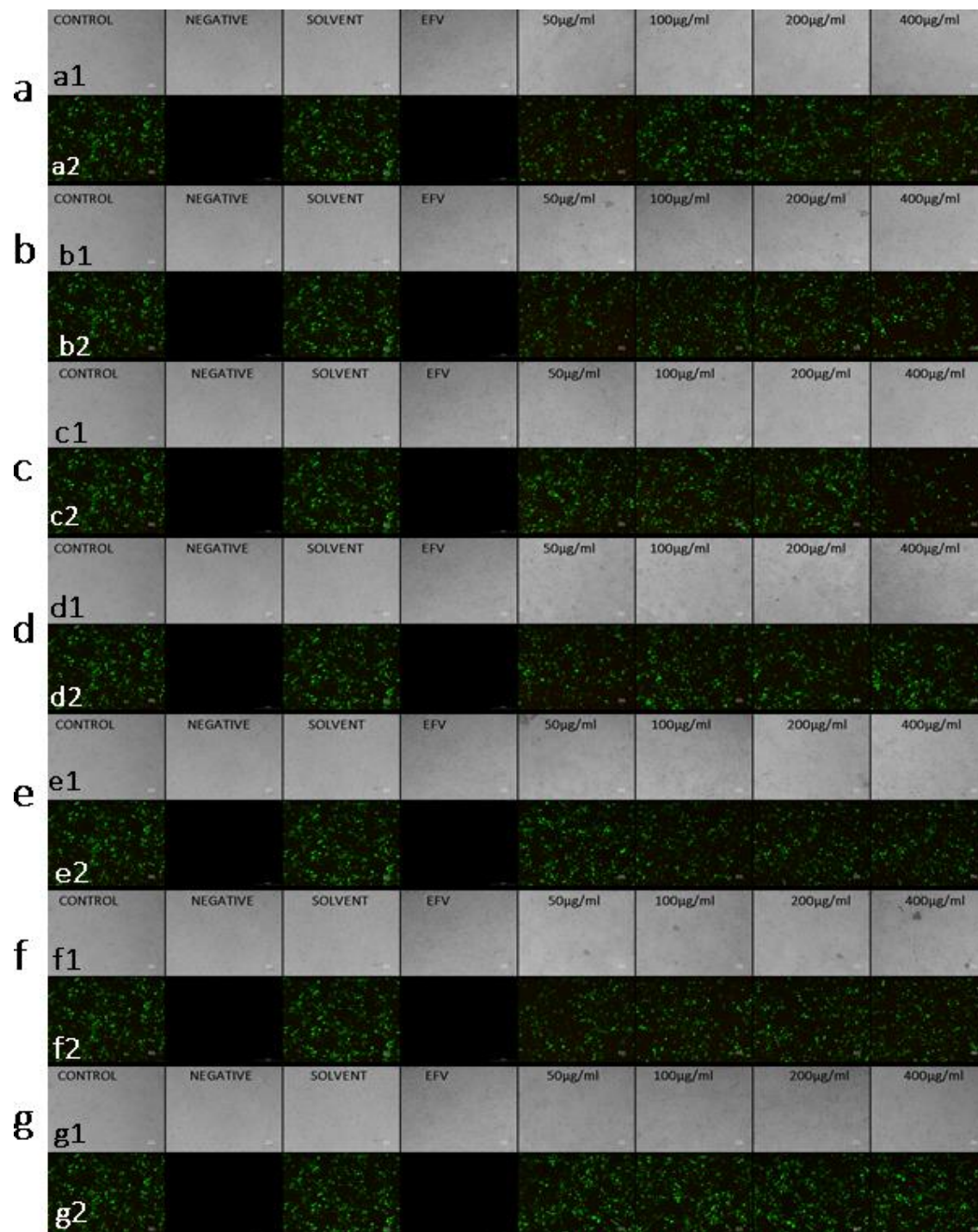
Supplementary data, Figure 1: Effect of crude methanolic fraction of *P. guajava* leaf extracts on cell viability: The graph represents the percentage of viable cells after treatment with increasing concentrations of the extracts (12.5µg/ml, 25µg/ml, 50µg/ml, 100µg/ml, 200µg/ml, 400µg/ml). Cell viability is expressed as percentage as compared to the control sets of the experiment. The CC_{50} value is 268.01µg/ml. All the sets were taken in triplicates; the data represent mean±S.D; p value <0.05; p value <0.01 versus control is considered statistically significant. * = p value <0.05, ** = p value <0.01.



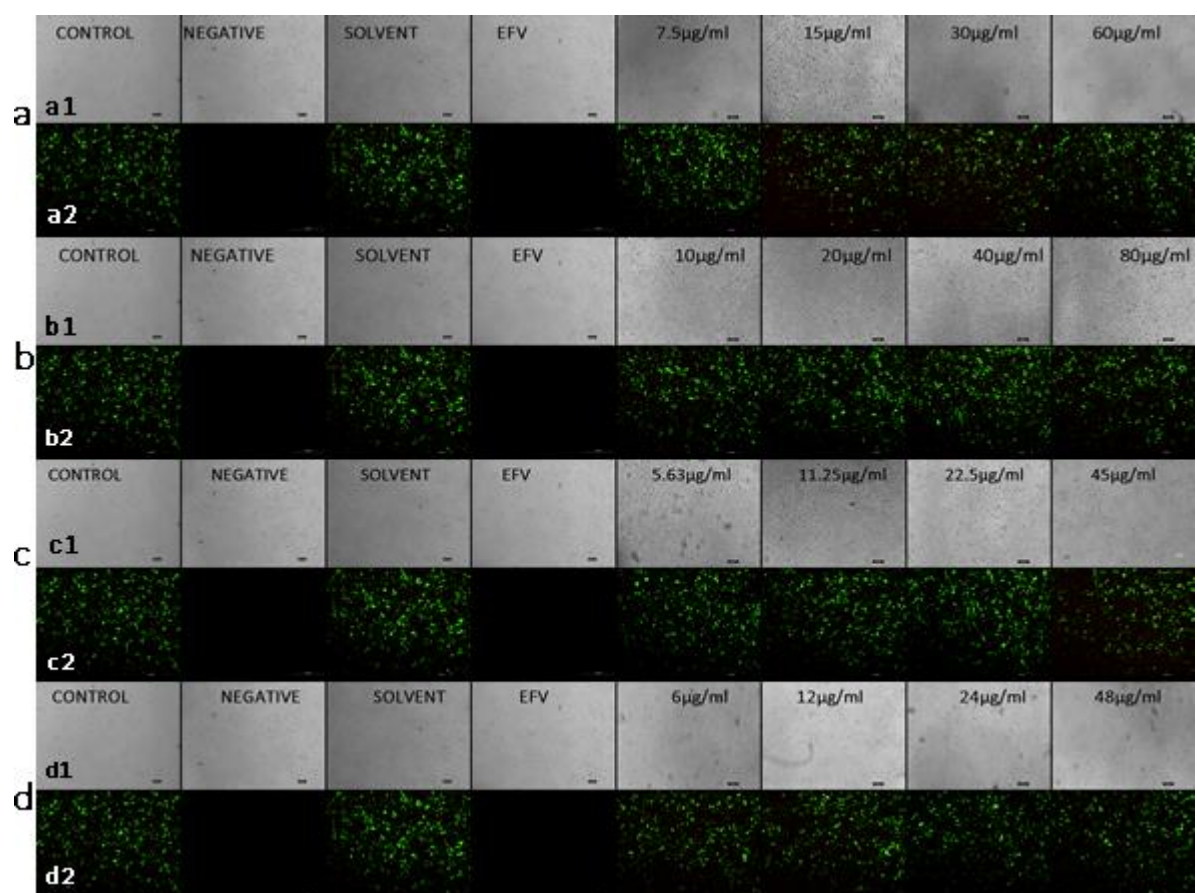
Supplementary data, Figure 2: Anti HIV activity of PB, EAc, Met fractions ((a)-PB, (b)-EAc, (c)Met) from *P.guajava* extract: Sub fractions PB and EAc obtained on solvent fractionation from the crude methanolic extract showed reduction in the GFP positive foci with increasing drug concentrations. The Met fraction however did not show any viral inhibition. The upper panels (a1,b1,c1) and lower panels (a2,b2,c2) indicate the bright field and fluoresce fields respectively (10X).



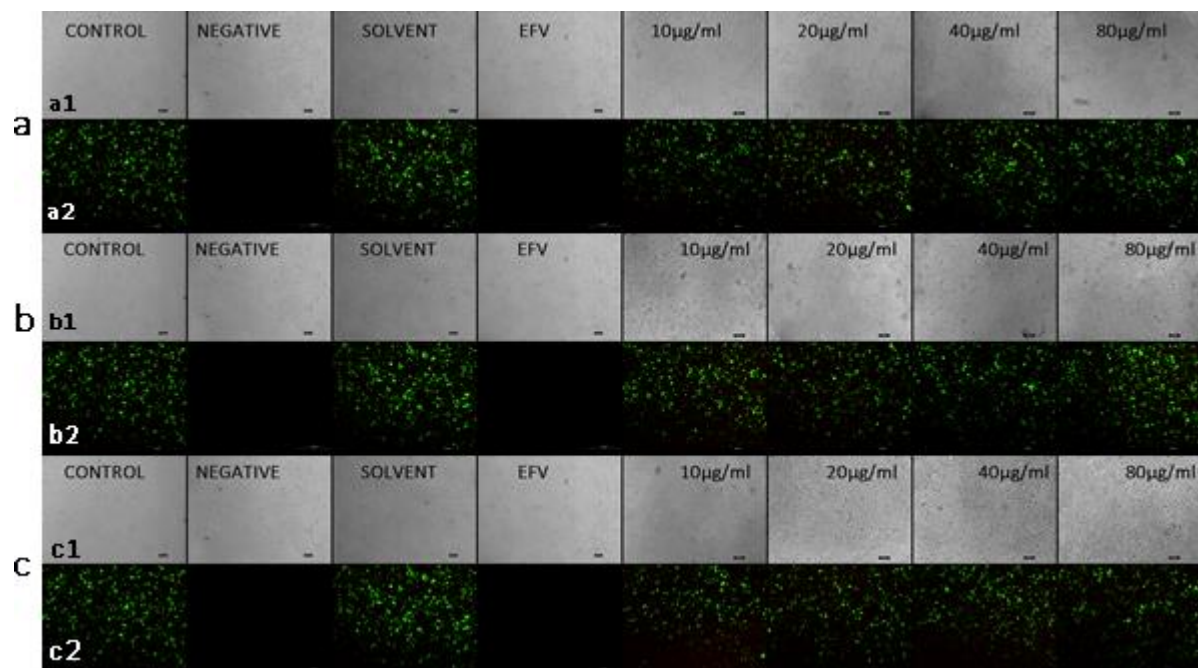
Supplementary data, Figure 3: Anti HIV activity of *P.guajava* extract (PB fractions-(P1-P7)): Huh 7 cells transduced with HIV-1 pseudovirus were treated with four different concentrations of the extracts for 48hours. Post treatment cells were visualized under fluorescent microscope. With increasing concentration, fraction P6 shows reduction in the GFP positive foci (f). Other fractions isolated from silica gel chromatography did not show significant inhibition of viral replication. The upper panel (a1, b1, c1, d1, e1, f1, g1) and lower panels(a2, b2, c2, d2, e2, f2, g2) indicate the bright field and fluorescence fields for the fraction respectively (10X).



Supplementary data, Figure 4: Anti HIV activity of *P.guajava* extract (EAc fractions-(E1-E7)): Huh 7 cells transduced with HIV-1 pseudovirus were treated with four different concentrations of the extracts for 48hours. Post treatment cells were visualized under fluorescent microscope. With increasing concentration, fraction E3 shows reduction in the GFP positive foci(c). Other fractions isolated from silica gel chromatography did not show significant inhibition of viral replication. The upper and lower panels indicate the bright field and fluorescence fields for the fraction respectively (10X).



Supplementary data, Figure 5: Anti HIV activity of semi purified fractions ((a)-A1, (b)-A3, (c)-A4, (d)-A5) from *P.guajava* extract: Sub fractions A(1-5) obtained on bioassay guided fractionation, as described in figure 1 were tested for their antiviral efficacy in cell culture. Infected Huh 7 cells were treated with four different concentrations of the drugs for 48 hours. Post treatment cells were visualized under fluorescent microscope. GFP expression analysis of the drug treated (A1, A3, A4, A5) cells shows no reduction in GFP positive foci in cells, indicating no inhibition of viral replication. The upper and lower panels indicate the bright field and fluorescence fields respectively (10X).



Supplementary data, Figure 6: Anti HIV activity of semi purified fractions ((a)-B1, (b)-B2, (c)-B3) from *P. guajava* extract: Sub fractions B(1-3) obtained on bioassay guided fractionation as described in figure 1, were tested for their antiviral efficacy in cell culture. Infected Huh 7 cells were treated with four different concentrations of the drugs for 48 hours. Post treatment cells were visualized under fluorescent microscope. GFP expression analysis of the drug treated (B1, B3, B4) cells show no reduction in GFP positive foci in cells, indicating no inhibition of viral replication. The upper and lower panels indicate the bright field and fluorescence fields respectively (10X).

Supplementary Table 1: Binding energies (kcal/mol) of compounds determined by molecular docking against HIV-1 RT. Compounds showing high or comparable binding energy compared to the control are represented in bold.

List of Compounds	Binding Energy (kcal/mol)
Efavirenz (positive control)	-6.2
Zidovudine(positive control)	-6.3
Norfloxacin(mock control)	-5.0
Compounds identified by HR-LCMS	
18-acetoxy-PGF2alpha-11-acetate	-11.4
Irigenindibenzyl ether	-8.6
Colforsin	-7.9
Deoxygedunol acetate	-7.5
Dihydromyricetin	-7.1
Dihydrodeoxystreptomycin	-6.4
Bromo-3-hydroxy-4-(succinyl-2-yl)-caryolane gamma-lactone	-6
1-Phosphatidyl-1D-myoinositol3-phosphate	-5.9
Fendiline	-5.4
Gln Ile Ala	-5.4
11-amino-undecanoic acid	-3.4