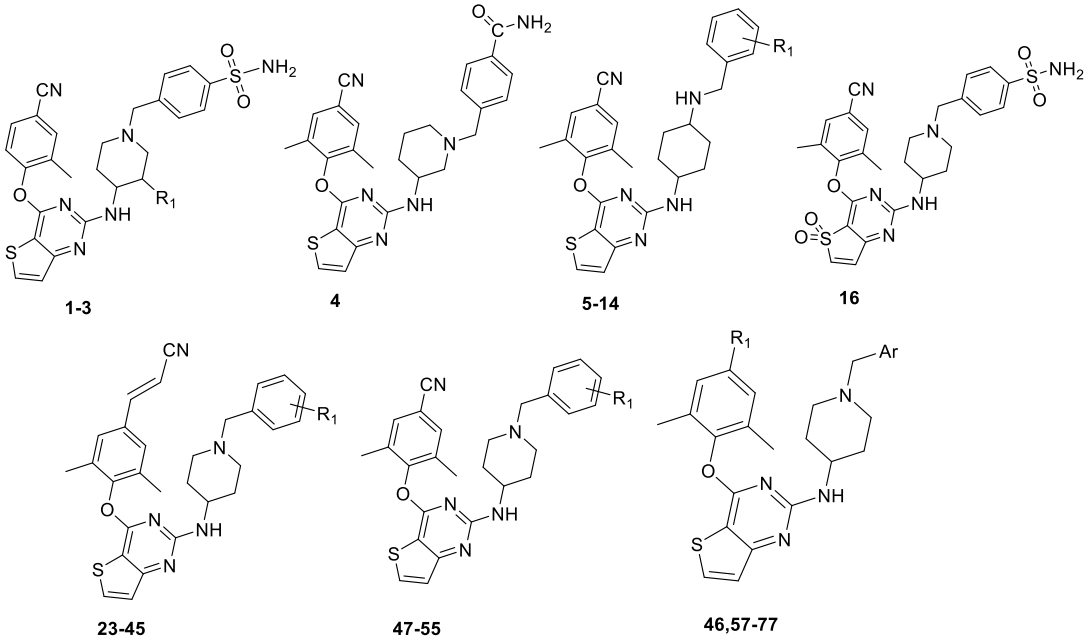
Table S1: Structures and anti-HIV Activity of all compounds.



No.	Structure		pEC_{50}	Predicted values		
	R_1	Ar		CoMFA	CoMSIA	T-CoMFA
1	F		8.24	8.27	8.37	8.24
2	$CO_2C_2H_5$		6.87	7.01	6.90	6.83
3	COOH		6.14	6.12	6.04	6.19
4			5.49	5.43	5.49	5.50
5	4-SO_2NH_2		7.37	7.46	7.36	7.40
6*	4-$CONH_2$		6.92	7.24	6.80	6.79
7*	3-$CONH_2$		6.87	6.80	6.49	6.20
8	4-NO_2		7.00	6.77	7.01	6.98
9	4-SO_2CH_3		7.24	7.23	7.29	7.24
10	H		6.64	6.48	6.44	6.65
11	4-Br		6.47	6.39	6.39	6.48
12	4-F		6.26	6.32	6.46	6.28
13	4-OH		5.88	6.00	5.98	5.82
14	3-CF_3		6.76	6.84	6.72	6.77
16			8.42	8.33	8.36	8.56
23	4-SO_2NH_2		8.91	8.76	8.96	8.80
24	4-SO_2CH_3		8.91	8.76	8.96	8.80
25	4-$CONH_2$		8.63	8.91	8.67	8.75
26	3-$CONH_2$		8.90	8.80	9.02	8.88
27	4-$COOC_2H_5$		8.49	8.51	8.50	8.55
28	4-F		7.84	7.80	7.84	7.91
29	3-F		8.23	8.11	7.92	8.15
30	2-F		8.01	8.05	7.96	8.12
31	4-Br		8.20	8.03	7.94	8.10
32*	3-Br		7.55	7.86	7.88	7.52
33*	2-Br		7.59	8.03	7.83	8.07
34	4-Cl		7.40	7.85	7.76	7.60
35*	3-Cl		7.59	7.85	7.89	7.65
36	2-Cl		7.59	8.03	7.88	8.07
37	4-NO_2		7.56	7.84	7.81	7.55
38	2-CH_3		8.11	7.97	8.16	8.12
39	4-CH_3		7.80	7.77	7.79	7.90
40	4-CN		8.05	7.93	7.90	8.11
41	3-CN		8.28	8.15	8.14	8.23

42	2-CN		8.35	8.36	8.29	8.34
43	Pyridine-4-yl		8.02	8.09	8.07	8.11
44	Pyridine-3-yl		8.48	8.28	8.12	8.21
45	Pyridine-2-yl		8.49	8.47	8.40	8.51
47	4-CN		8.47	8.49	8.52	8.47
48	2-CN		8.84	8.77	8.71	8.82
49	4-Br		8.23	8.17	8.21	8.25
50	2-CH_3		8.24	8.26	8.21	8.13
51	3-CN		7.58	7.92	7.99	7.54
52*	4-$COOCH_3$		8.03	7.93	7.86	7.92
53	3-F		8.38	8.42	8.41	8.36
54	2-F		8.49	7.94	7.99	8.34
55	4-NO_2		8.36	8.30	8.07	8.14
46	CN	4-SO_2NH_2-Ph	8.08	8.11	8.09	8.12
57	CN	4-F-Ph	8.12	8.05	8.10	8.14
58	CN	Pyridine-4-yl	8.12	8.07	8.01	8.17
59*	CN	2,4-diF-Ph	7.99	8.15	8.11	8.24
60	CN	3-SO_2NH_2-Ph	7.66	8.22	8.06	8.10
61	CN	4-$NHSO_2Me$-Ph	8.62	8.56	8.58	8.59
62*	CN	4-SO_2NHMe-Ph	8.82	8.79	8.83	8.86
63*	CN	4-$CONH_2$-Ph	8.82	8.85	8.58	8.64
64	CN	3-$CONH_2$-Ph	8.85	7.90	8.25	8.90
66*	CN	4-$SO_2NHCOMe$-Ph	8.60	8.58	8.63	8.57
67	CH_3	4-SO_2Me-Ph	8.28	9.10	9.31	8.48
68	CH_3	4-CO_2Me-Ph	8.24	8.20	8.25	8.13
69*	CH_3	4-F-Ph	7.81	7.90	7.91	7.70
70	CH_3	3-F-Ph	7.59	7.25	7.41	7.53
71	CH_3	3-CN-Ph	7.41	7.46	7.46	7.50
72*	CH_3	Pyridine-4-yl	7.68	7.60	7.77	7.72
73	CH_3	2,4-diF-Ph	8.12	7.40	7.47	7.59
74	CH_3	4-$CONH_2$-Ph	7.43	7.53	7.44	7.46
75*	CH_3	3-$CONH_2$-Ph	8.19	8.22	8.20	8.26
77	CH_3	4-NO_2-Ph	7.84	7.80	7.99	7.93

The compound labeled with "*" is the test set.

Table S2: 31 possible combinations of CoMSIA molecular fields (Alignment Ⅰ).

CoMSIA	*LOO*		*PLS*			*Normalized Coefficients*				
	n	q^2	r^2	*SEE*	*F*	*S*	*E*	*H*	*D*	*A*
S	*4*	*0.484*	*0.804*	*0.362*	*50*	*1*				
E	*2*	*0.378*	*0.677*	*0.456*	*53*		*1*			
H	*12*	*0.34*	*0.966*	*0.165*	*96*			*1*		
D	*3*	*0.284*	*0.752*	*0.403*	*50*				*1*	
A	*8*	*0.532*	*0.861*	*0.318*	*34*					*1*
S+E	*6*	*0.423*	*0.933*	*0.216*	*109*	*0.158*	*0.842*			
S+H	*12*	*0.453*	*0.971*	*0.152*	*115*	*0.284*		*0.716*		
S+D	*12*	*0.413*	*0.930*	*0.236*	*45*	*0.444*			*0.556*	
S+A	*6*	*0.619*	*0.914*	*0.244*	*86*	*0.240*				*0.760*
E+H	*5*	*0.409*	*0.910*	*0.248*	*96*		*0.678*	*0.322*		
E+D	*4*	*0.32*	*0.868*	*0.298*	*80*		*0.467*		*0.533*	
E+A	*6*	*0.624*	*0.946*	*0.194*	*138*		*0.551*			*0.449*
H+D	*3*	*0.3*	*0.768*	*0.390*	*55*			*0.305*	*0.695*	
H+A	*6*	*0.507*	*0.925*	*0.229*	*95*			*0.373*		*0.627*
D+A	*9*	*0.541*	*0.955*	*0.184*	*102*				*0.416*	*0.584*
S+E+H	*5*	*0.453*	*0.906*	*0.253*	*92*	*0.122*	*0.589*	*0.289*		
S+E+D	*4*	*0.357*	*0.878*	*0.285*	*88*	*0.081*	*0.432*		*0.487*	
S+E+A	*6*	*0.604*	*0.948*	*0.19*	*143*	*0.098*	*0.472*			*0.429*
S+H+D	*4*	*0.34*	*0.812*	*0.355*	*52*	*0.109*		*0.278*	*0.613*	
S+H+A	*6*	*0.556*	*0.927*	*0.225*	*99*	*0.139*		*0.291*		*0.510*
S+D+A	*9*	*0.551*	*0.956*	*0.18*	*107*	*0.073*			*0.387*	*0.539*
E+H+D	*4*	*0.37*	*0.893*	*0.267*	*102*		*0.384*	*0.193*	*0.423*	
E+H+A	*7*	*0.574*	*0.961*	*0.166*	*162*		*0.4*	*0.221*		*0.379*
E+D+A	*6*	*0.523*	*0.957*	*0.174*	*173*		*0.323*		*0.327*	*0.350*
H+D+A	*9*	*0.509*	*0.965*	*0.161*	*135*			*0.214*	*0.348*	*0.438*
S+E+H+D	*4*	*0.407*	*0.903*	*0.255*	*113*	*0.065*	*0.358*	*0.184*	*0.393*	
S+E+H+A	*7*	*0.579*	*0.962*	*0.165*	*165*	*0.075*	*0.369*	*0.199*		*0.357*
S+E+D+A	*6*	*0.529*	*0.957*	*0.173*	*174*	*0.048*	*0.307*		*0.307*	*0.338*
S+H+D+A	*7*	*0.524*	*0.956*	*0.17*	*142*	*0.062*		*0.166*	*0.356*	*0.416*
E+H+D+A	*7*	*0.516*	*0.965*	*0.157*	*182*		*0.278*	*0.135*	*0.281*	*0.305*
S+E+H+D+A	*7*	*0.528*	*0.966*	*0.157*	*184*	*0.044*	*0.266*	*0.131*	*0.266*	*0.292*

Table S2: 31 possible combinations of CoMSIA molecular fields (Alignment II).

CoMSIA	*LOO*		*PLS*			*Normalized Coefficients*				
	n	q^2	r^2	*SEE*	*F*	*S*	*E*	*H*	*D*	*A*
S	*3*	*0.461*	*0.728*	*0.422*	*44*	*1*				
E	*1*	*0.268*	*0.427*	*0.601*	*38*		*1*			
H	*3*	*0.257*	*0.676*	*0.461*	*34*			*1*		
D	*3*	*0.272*	*0.741*	*0.412*	*47*				*1*	
A	*8*	*0.554*	*0.900*	*0.27*	*50*					*1*
S+E	*1*	*0.300*	*0.460*	*0.583*	*44*	*0.196*	*0.804*			
S+H	*10*	*0.429*	*0.963*	*0.167*	*112*	*0.272*		*0.728*		
S+D	*10*	*0.394*	*0.918*	*0.250*	*47*	*0.346*			*0.654*	
S+A	*7*	*0.636*	*0.929*	*0.225*	*85*	*0.221*				*0.779*
E+H	*10*	*0.320*	*0.984*	*0.111*	*261*		*0.614*	*0.386*		
E+D	*1*	*0.282*	*0.518*	*0.551*	*55*		*0.485*		*0.515*	
E+A	*6*	*0.556*	*0.952*	*0.184*	*154*		*0.501*			*0.499*
H+D	*4*	*0.297*	*0.795*	*0.371*	*47*			*0.295*	*0.705*	
H+A	*6*	*0.542*	*0.924*	*0.231*	*94*			*0.365*		*0.635*
D+A	*10*	*0.574*	*0.957*	*0.181*	*95*				*0.413*	*0.587*
S+E+H	*10*	*0.391*	*0.983*	*0.112*	*255*	*0.099*	*0.551*	*0.350*		
S+E+D	*4*	*0.301*	*0.894*	*0.267*	*102*	*0.081*	*0.440*		*0.479*	
S+E+A	*6*	*0.563*	*0.954*	*0.179*	*162*	*0.088*	*0.446*			*0.466*
S+H+D	*5*	*0.327*	*0.879*	*0.288*	*69*	*0.103*		*0.282*	*0.615*	
S+H+A	*6*	*0.572*	*0.926*	*0.227*	*98*	*0.132*		*0.292*		*0.576*
S+D+A	*9*	*0.573*	*0.957*	*0.180*	*107*	*0.070*			*0.404*	*0.527*
E+H+D	*6*	*0.298*	*0.947*	*0.193*	*138*		*0.421*	*0.188*	*0.391*	
E+H+A	*6*	*0.569*	*0.954*	*0.179*	*162*		*0.362*	*0.208*		*0.430*
E+D+A	*6*	*0.507*	*0.960*	*0.168*	*185*		*0.306*		*0.341*	*0.353*
H+D+A	*10*	*0.542*	*0.970*	*0.152*	*137*			*0.327*	*0.339*	*0.434*
S+E+H+D	*7*	*0.342*	*0.964*	*0.159*	*178*	*0.066*	*0.399*	*0.189*	*0.345*	
S+E+H+A	*6*	*0.571*	*0.956*	*0.175*	*169*	*0.070*	*0.193*	*0.337*		*0.401*
S+E+D+A	*6*	*0.519*	*0.961*	*0.166*	*190*	*0.049*	*0.291*		*0.322*	*0.338*
S+H+D+A	*10*	*0.559*	*0.970*	*0.152*	*136*	*0.060*		*0.217*	*0.318*	*0.404*
E+H+D+A	*7*	*0.515*	*0.969*	*0.149*	*205*		*0.263*	*0.130*	*0.287*	*0.320*
S+E+H+D+A	*10*	*0.520*	*0.981*	*0.121*	*221*	*0.041*	*0.279*	*0.160*	*0.228*	*0.292*