Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Materials

Exploring the binding mode of HIV-1 Vif inhibitors by blind docking, molecular dynamics and MM/GBSA

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Binding free energies and individual energy terms of five compounds are listed in Table S1. The correlation between the experimental and the calculated pIC_{50} of eleven binding modes are shown in Figure S1.

Table S1. Binding free energies and individual energy terms of five compounds.

Compound **1**					
Residue	ΔG_{vdw}	ΔG_{ele}	ΔG_{GB}	ΔG_{SA}	$\Delta G_{residue\text{-}inhibitor}$
GLN 136	–1.10	–0.17	–0.20	–0.26	–1.72
ALA 137	–0.21	–0.12	0.06	–0.05	–0.31
GLY 138	–0.39	–0.03	–0.02	–0.09	–0.52
HIS 139	–2.06	–0.01	–0.09	–0.33	–2.48
SER 144	–0.70	–0.35	0.15	–0.19	–1.08
TYR 147	–1.08	0.51	–0.37	–0.19	–1.13
LEU 148	–0.42	0.01	–0.01	–0.11	–0.53
LEU 150	–0.98	–0.29	–0.09	–0.16	–1.51
ALA 151	–1.77	0.38	–0.36	–0.23	–1.98
ILE 154	–0.76	–0.14	0.05	–0.17	–1.02
THR 155	–1.55	–0.07	0.01	–0.28	–1.89
LYS 176	–0.64	–1.86	1.50	–0.14	–1.13
PRO 177	–1.11	0.57	–0.50	–0.19	–1.22
Compound **2**					
Residue	ΔG_{vdw}	ΔG_{ele}	ΔG_{GB}	ΔG_{SA}	$\Delta G_{residue\text{-}inhibitor}$
GLN 136	–0.70	–0.24	–0.48	–0.16	–1.57
GLY 138	–1.70	–0.66	–0.15	–0.26	–2.78
HIS 139	–1.55	–0.74	0.53	–0.24	–2.00
ASN 140	–1.51	–0.02	–0.2	–0.28	–2.00
TYR 147	–2.63	0.17	–0.18	–0.36	–3.00
LEU 148	–0.77	0.11	–0.09	–0.24	–0.99
LEU 150	–0.81	0.06	–0.18	–0.15	–1.08
ALA 151	–1.53	0.35	–0.39	–0.24	–1.81
ILE 154	–0.50	–0.15	0.08	–0.11	–0.67
THR 155	–1.22	–0.49	0.35	–0.30	–1.65
ILE 159	–0.60	–0.20	0.18	–0.14	–0.72
ARG 173	–0.45	–2.40	2.21	–0.09	–0.74
PRO 177	–1.11	–3.24	2.60	–0.20	–1.95
Compound **3**					
Residue	ΔG_{vdw}	ΔG_{ele}	ΔG_{GB}	ΔG_{SA}	$\Delta G_{residue\text{-}inhibitor}$
GLN 136	–1.89	–1.80	0.46	–0.43	–3.66
ALA 137	–1.49	–1.07	0.42	–0.19	–2.33
GLY 138	–1.65	–1.15	0.45	–0.20	–2.55
HIS 139	–2.53	–1.60	0.06	–0.31	–4.37
ASN 140	–0.68	–0.89	0.39	–0.70	–1.28
LYS 141	–1.08	–1.26	0.47	–0.20	–2.07
VAL 142	–0.37	0.24	–0.21	–0.07	–0.41
TYR 147	–1.90	–0.20	0.04	–0.25	–2.31
LEU 148	–1.37	0.31	–0.35	–0.32	–1.73
LEU 150	–1.25	0.95	–0.82	–0.20	–1.31
ALA 151	–2.39	0.59	–0.59	–0.25	–2.64

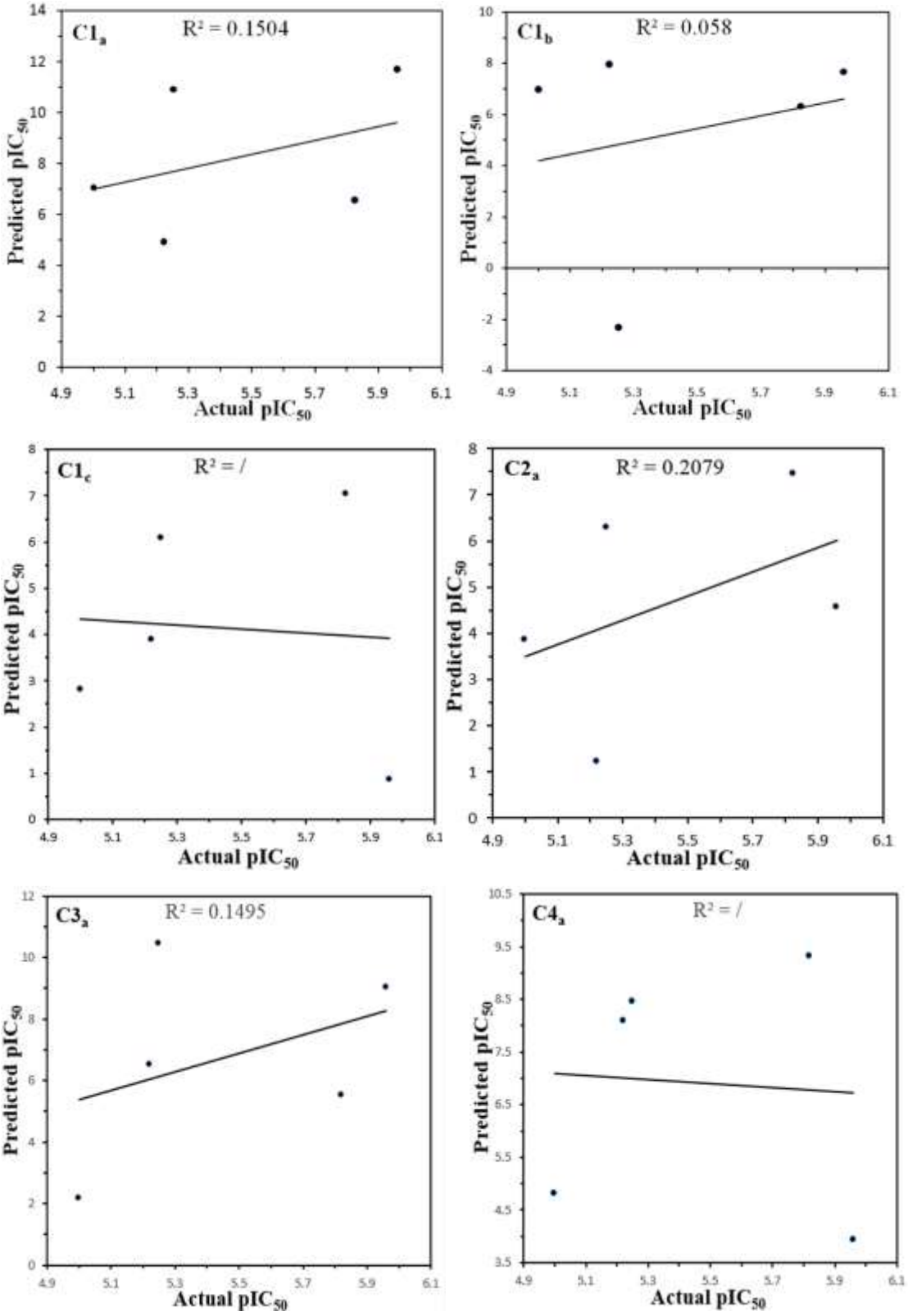
ILE 154	–0.78	–0.55	0.24	–0.20	–1.29

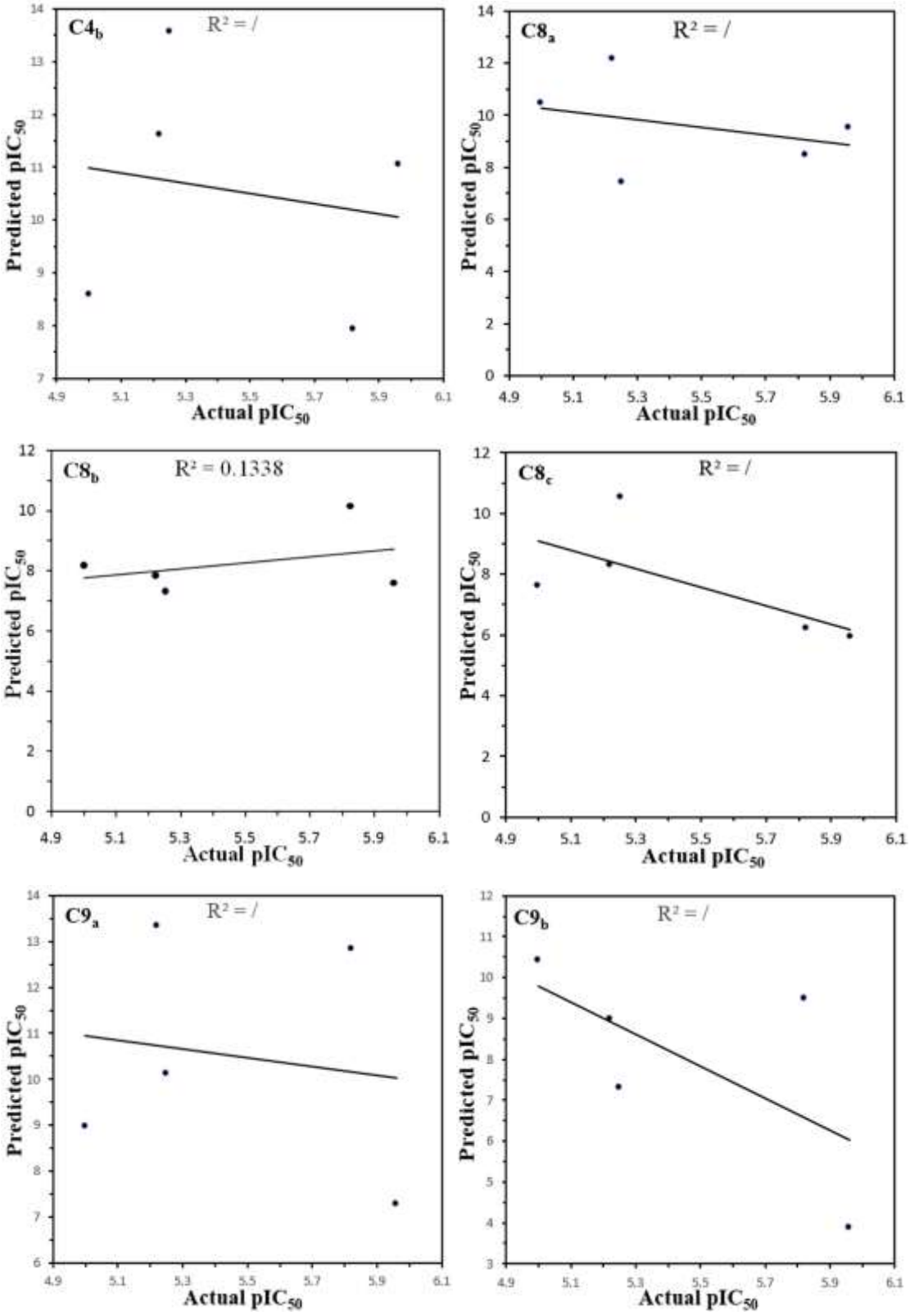
Compound **4**

Residue	ΔG_{vdw}	ΔG_{ele}	ΔG_{GB}	ΔG_{SA}	$\Delta G_{residue\text{-}inhibitor}$
GLN 136	–0.53	–0.24	0.16	–0.16	–0.77
HIS 139	–0.49	–0.25	0.20	–0.07	–0.61
ASN 140	–1.97	–0.78	0.04	–0.35	–3.06
LYS 141	–1.03	–1.94	1.60	–0.16	–1.52
VAL 142	–0.57	0.19	–0.20	–0.19	–0.77
TYR 147	–1.50	–0.06	–0.17	–0.24	–1.97
LEU 148	–1.68	0.13	–0.13	–0.33	–2.01
LEU 150	–1.09	–0.52	0.12	–0.20	–1.66
ALA 151	–2.29	–0.15	0.05	–0.28	–2.67
ALA 152	–0.57	–0.02	0.11	–0.13	–0.62
ILE 154	–0.48	–0.19	0.10	–0.13	–0.70
THR 155	–0.41	0.07	–0.08	–0.13	–0.55
LYS 176	–0.27	–2.01	1.81	–0.09	–0.57

Compound **5**

Residue	ΔG_{vdw}	ΔG_{ele}	ΔG_{GB}	ΔG_{SA}	$\Delta G_{residue\text{-}inhibitor}$
GLU 134	–0.42	–1.26	1.12	–0.17	–0.74
GLN 136	–2.42	–1.00	0.58	–0.35	–3.19
ALA 137	–1.11	0.01	–0.02	–0.19	–1.30
GLY 138	–1.12	0.26	–0.05	–0.16	–1.07
HIS 139	–0.39	–0.01	0.02	–0.06	–0.44
LYS 141	–0.35	0.15	–0.17	–0.10	–0.48
GLY 143	–0.44	0.13	–0.04	–0.16	–0.52
SER 144	–0.32	–0.80	0.59	–0.06	–0.60
TYR 147	–3.07	–0.83	0.65	–0.45	–3.71
LEU 148	–1.32	0.33	–0.35	–0.32	–1.66
LEU 150	–0.97	0.34	–0.42	–0.20	–1.23
ALA 151	–2.29	0.07	–0.22	–0.25	–2.70
ILE 154	–1.14	–0.13	0.15	–0.23	–1.35
THR 155	–0.84	–0.27	0.28	–0.23	–1.07
LYS 176	–0.97	–0.24	0.15	–0.17	–1.23
PRO 177	–1.69	–1.78	1.10	–0.22	–2.58





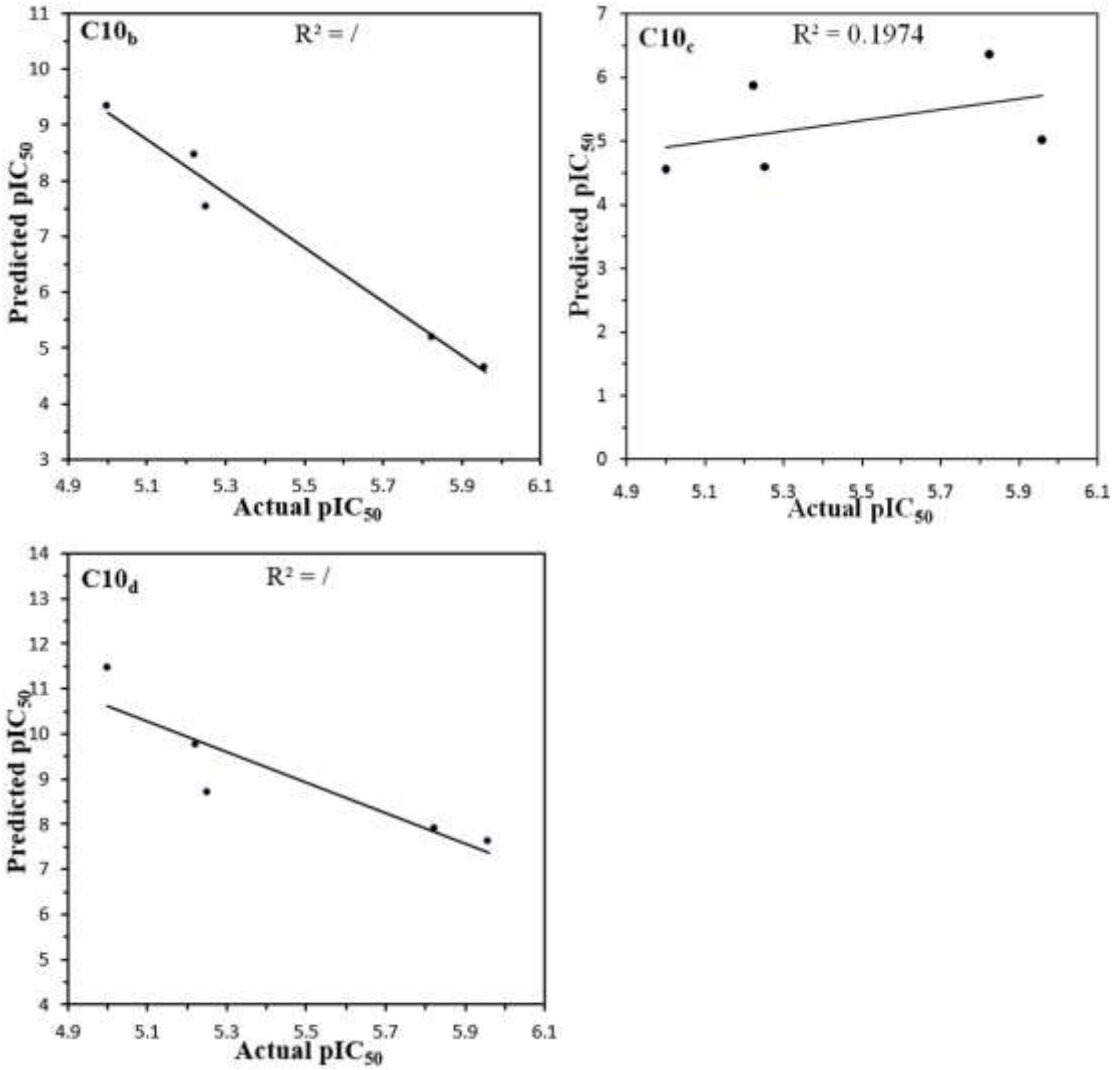


Figure S1. The correlation between the experimental and the calculated pIC_{50} of fifteen binding modes.