

Supplementary Material

Quantum Mechanics/Molecular Mechanics Study on Caspase-2 Recognition by Peptide Inhibitors

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Table S1. QM/MM binding free energies for caspase-2:peptide complexes

Complex ^(a)	$\Delta G_{\text{bind}}^{(b)}$ (kcal mol ⁻¹)	ΔH (kcal mol ⁻¹)	$T\Delta S_{\text{total}}$ (kcal mol ⁻¹)	$T\Delta S_{\text{trans}}$ (kcal mol ⁻¹)	$T\Delta S_{\text{rot}}$ (kcal mol ⁻¹)	$T\Delta S_{\text{sb}}$ (kcal mol ⁻¹)
casp-2:VDVAD	-13.22	-31.85	-18.63	-12.90	-10.61	4.88
casp-2:VDVAE	-6.01	-26.98	-20.97	-12.93	-10.74	2.70
casp-2:VEVAD	-11.57	-29.60	-18.03	-12.93	-10.62	5.52
casp-2:VEVAE	-7.11	-29.76	-22.65	-12.96	-10.98	1.29
casp-2:VDVGD	-2.82	-30.84	-28.02	-12.90	-10.95	-4.17
casp-2:VEVGd	-0.13	-30.98	-30.85	-12.90	-10.48	-7.47
casp-2:VDVGE	-3.15	-26.76	-23.61	-12.90	-10.86	0.15
casp-2:VEVGE	-0.75	-29.58	-28.83	-12.93	-10.95	-4.95
casp-2:LDVAD	-7.05	-28.50	-21.45	-12.90	-10.74	2.19
casp-2:LDVAE	-4.11	-25.74	-21.63	-12.96	-10.83	2.16
casp-2:LEVAD	-3.71	-29.03	-25.32	-12.93	-10.92	-1.47
casp-2:LEVAE	-2.73	-27.75	-25.02	-12.93	-11.04	-1.05
casp-2:LDVGD	-4.29	-30.66	-26.37	-12.90	-10.83	-2.64
casp-2:LEVGD	-1.78	-30.01	-28.23	-12.90	-11.01	-4.32
casp-2:LDVGE	-0.34	-25.81	-25.47	-12.93	-10.89	-1.65
casp-2:LEVGE	-3.89	-27.77	-23.88	-12.96	-10.86	-0.06
casp-2:VDLAD	-9.27	-29.52	-20.25	-12.90	-10.65	3.30
casp-2:VDLAE	-11.09	-29.12	-18.03	-12.93	-10.59	5.49
casp-2:VELAD	-13.84	-33.49	-19.65	-12.93	-10.71	3.99
casp-2:VELAE	-5.79	-31.17	-25.38	-12.93	-10.86	-1.59
casp-2:VDLGD	-4.35	-30.78	-26.43	-12.90	-10.95	-2.58
casp-2:VELGD	-5.62	-32.41	-26.79	-12.90	-11.07	-2.82
casp-2:VDLGE	-10.52	-28.82	-18.30	-12.93	-10.65	5.28
casp-2:VELGE	-9.33	-28.38	-19.05	-12.96	-10.89	4.80
casp-2:LDLAD	-5.58	-27.54	-21.96	-12.93	-10.71	1.68
casp-2:LDLAE	-1.83	-26.87	-25.04	-12.98	-10.98	-1.08
casp-2:LELAD	-9.75	-32.91	-23.16	-12.93	-10.83	0.60
casp-2:LELAE	-8.55	-29.13	-20.58	-12.96	-10.89	3.27
casp-2:LDLGD	-2.03	-29.36	-27.33	-12.90	-11.07	-3.36
casp-2:LELGD	-4.40	-30.65	-26.25	-12.93	-11.07	-2.25
casp-2:LDLGE	-3.42	-25.68	-22.26	-12.90	-10.68	1.32
casp-2:LELGE	-4.45	-27.64	-23.19	-12.93	-10.83	0.57
casp-2:IDVAD	-10.72	-29.35	-18.63	-12.90	-10.65	4.92
casp-2:IDVAE	-1.15	-26.80	-25.65	-12.93	-10.95	-1.77
casp-2:IEVAD	-7.06	-29.53	-22.47	-12.93	-10.77	1.23
casp-2:IEVAE	-5.04	-33.48	-28.44	-12.93	-11.16	-4.35
casp-2:IDVGD	-2.76	-30.09	-27.33	-12.90	-10.86	-3.57
casp-2:IEVGd	-4.02	-29.31	-25.29	-12.90	-10.89	-1.50
casp-2:IDVGE	-4.48	-27.37	-22.89	-12.93	-10.77	0.81
casp-2:IEVGE	-6.15	-32.64	-26.49	-12.96	-11.01	-2.52
casp-2:VDIAD	-11.45	-32.75	21.30	-12.90	-10.68	2.28
casp-2:VDIAE	-3.35	-27.35	-24.00	-12.90	-10.89	-0.21
casp-2:VEIAD	-12.64	-30.91	-18.27	-12.93	-10.56	5.22
casp-2:VEIAE	-0.80	-30.26	-29.46	-12.93	-10.89	-5.64
casp-2:VDIGD	-1.64	-31.79	-30.15	-12.90	-10.98	-6.27
casp-2:VEIGD	-3.73	-31.99	-28.26	-12.90	-11.01	-4.35
casp-2:VDIGE	-5.62	-26.80	-21.18	-12.93	-10.71	2.46
casp-2:VEIGE	-10.21	-29.29	-19.08	-12.96	-10.71	4.59

casp-2:IDIAD	-9.80	-29.63	-19.83	-12.93	-10.68	3.78
casp-2:IDIAE	-7.99	-27.16	-19.17	-12.93	-10.65	4.41
casp-2:IEIAD	-10.85	-26.60	-15.75	-12.78	-10.32	7.35
casp-2:IEIAE	-7.78	-33.07	-25.29	-12.96	-11.07	-1.26
casp-2:IDIGD	-3.48	-31.47	-27.99	-12.90	-10.89	-4.20
casp-2:IEIGD	-5.44	-31.48	-26.04	-12.93	-10.92	-2.19
casp-2:IDIGE	-5.95	-26.92	-20.97	-12.96	-10.77	2.76
casp-2:IEIGE	-10.01	-33.26	-23.25	-12.93	-11.01	0.69
casp-2:LDIAD	-10.54	-31.87	-21.33	-12.93	-10.65	2.25
casp-2:LDIAE	-7.18	-25.90	-18.72	-13.05	-10.65	4.98
casp-2:LEIAD	-8.08	-31.80	-23.72	-12.93	-10.94	0.15
casp-2:LEIAE	-7.20	-27.78	-20.58	-12.96	-10.89	3.27
casp-2:LDIGD	-0.04	-30.99	-30.95	-12.80	-11.13	-7.02
casp-2:LEIGD	-3.31	-31.72	-28.41	-12.93	-10.89	-4.59
casp-2:LDIGE	-3.24	-25.17	-21.93	-12.96	-10.74	1.77
casp-2:LEIGE	-3.70	-27.79	-24.09	-12.93	-10.80	-0.36
casp-2:IDLAD	-10.07	-29.96	-19.89	-12.93	-10.59	3.63
casp-2:IDLAE	-4.98	-28.14	-23.16	-12.93	-10.95	0.72
casp-2:IELAD	-6.21	-28.26	-22.05	-12.93	-10.68	1.56
casp-2:IELAE	-7.38	-28.89	-21.51	-12.96	-10.77	2.22
casp-2:IDLGD	-0.20	-27.41	-27.21	-12.90	-10.95	-3.36
casp-2:IELGD	-2.39	-27.50	-25.11	-12.93	-10.95	-1.23
casp-2:IDLGE	-6.99	-27.12	-20.13	-12.96	-10.68	3.51
casp-2:IELGE	-3.31	-28.78	-25.47	-12.93	-10.83	-1.71

^(a) Ala (A), Asp (D), Glu (E), Gly (G), Ile (I), Leu (L), Val (V)

^(b) Gibb's free energy (ΔG), enthalpy (ΔH), entropy ($T\Delta S$) and entropic contribution, translational ($T\Delta S_{\text{trans}}$), rotational ($T\Delta S_{\text{rot}}$), vibrational ($T\Delta S_{\text{vib}}$) are derived from Eqs. 2 and 3.