RECOGNITION BY THYROID HORMONE RECEPTOR OF CANONICAL DNA RESPONSE ELEMENTS.

Ana Carolina Migliorini Figueira, Luís Maurício T. R. Lima, Leonardo H. F. Lima, Americo T. Ranzani, Guilherme dos Santos Mule and Igor Polikarpov

Supporting Information

Table I - Comparison between the χ^2 values for each of the applied models.

HRE	Without Mg^{2+}			With 1 mM Mg^{2+}		
	$\chi^2_{intermediate}$	χ^2_{2state}	$\chi^2_{cooperative}$	$\chi^2_{intermediate}$	χ^2_{2state}	$\chi^2_{cooperative}$
TR DBD-LBD F2	1.47583	2.85212	_____	_____	4.57751	_____
TR DBD-LBD PAL	2.96215	2.93942	_____	0.21923	0.29395	_____
TR DBD-LBD DR4	0.30622	0.28802	_____	0.98895	0.94141	_____
TR DBD-LBD DR1	0.58892	0.69123	_____	0.29981	0.30096	_____
TR DBD – F2	5.463509	5.73135	4.856228	2.171591	2.01354	3.83093
TR DBD - PAL	0.887477	0.77784	1.104324	2.808555	2.77857	2.413675
TR DBD - DR4	1.831825	1.60724	2.104373	1.624	1.29715	1.297153
TR DBD - DR1	167.7325	195.542	143.9	2.958015	2.90843	2.725714

Lower values indicate the best fitting. Nd- non determined.

Table II - ΔG values recovered by BIOEQS and Hill analyses.

		ΔG MD (kcal/mol*K)	err +	err -	ΔG MMD (kcal/mol*K)	err +	err -	ΔG MD2 (kcal/mol*K)	err +	err -	ΔG cooperative (kcal/mol*K)	err +	err -	ΔGapp Bioeqs (kcal/mol*K)	err +	err -	Δ Gapp Hill (kcal/mol*K)	err +/-
TR DBD with Mg	F2	10.51	0.45	0.6	20.1	0.41	0.37	9.91	0.2	0.19	ND	ND	ND	10.05	0.21	0.19	9.844	8×10^{-6}
	PAL	10.47	<11.8	0	21.44	0.25	1.02	10.2	0.41	0.37	20.92	0.66	0.49	10.72	0.09	0.08	10.041	6×10^{-6}
	DR4	1.22	<11.1	0	19.61	0.68	0.98	9.73	0.53	0.76	19.6	0.63	0.87	9.8	0.32	0.44	10.363	3×10^{-6}
	DR1	9.69	0.6	0.93	16.92	0.33	0.26	8.35	0.31	0.31	16.92	0.3	0.26	8.45	0.62	0.62	8.444	4×10^{-4}
TR DBD without Mg	F2	0.46	<11.4	0	9.8	0.69	0.69	20.32	1.19	0.61	20.32	1.19	0.61	10.15	0.62	0.41	9.723	1×10^{-5}
	PAL	9.47	0.76	2.5	18.25	0.64	0.72	8.99	0.4	0.4	18.44	0.9	0.72	9.12	0.32	0.36	9.358	4×10^{-5}
	DR4	9.86	<10.6	0	19.23	0.45	0.82	9.45	0.26	0.26	19.3	0.41	0.35	9.61	0.23	0.41	9.208	5×10^{-5}
	DR1	8.09	<9.01	0	17.07	0.31	0.36	8.48	0.27	0.31	17.06	0.26	0.31	8.53	0.16	0.18	8.402	4×10^{-4}
TR DBD-LBD with Mg	F2	ND	ND	ND	ND	ND	ND	11.77	0.66	0.47	ND	ND	ND	11.77	0.33	0.24	11.109	9×10^{-7}
	PAL	9.57	0.25	0.3	18.73	0.17	0.15	9.28	0.11	0.11	ND	ND	ND	9.38	0.62	0.62	9.235	4×10^{-5}
	DR4	9.56	0.48	0.41	18.03	0.36	0.32	8.99	0.2	0.19	ND	ND	ND	9.01	0.18	0.16	9.001	9×10^{-5}
	DR1	9.69	0.6	0.93	17.38	<18.6		8.98	0.54	0.54	ND	ND	ND	8.69	0.09	0.08	8.545	2×10^{-4}
TR DBD-LBD without Mg	F2	11.44	1.04	0.74	20.2	1.09	0.82	9.73	0.53	0.63	ND	ND	ND	10.1	0.95	0.41	10.227	6×10^{-5}
	PAL	9.85	0.36	0.45	18.41	0.37	0.49	9.24	0.19	0.19	ND	ND	ND	9.20	0.33	0.31	9.379	3×10^{-5}
	DR4	9.72	0.46	1.05	18.96	0.44	0.39	9.37	0.22	0.22	ND	ND	ND	9.48	0.22	0.2	9.317	4×10^{-5}
	DR1	9.49	0.18	0.21	17.77	0.2	0.23	8.84	0.11	0.11	ND	ND	ND	8.885	0.1	0.12	8.790	4×10^{-3}

ΔG values are given in $kcal \cdot mol^{-1} K^{-1}$. **ΔG MD and ΔG MMD** dissociation free energies for the first (MD) and second (MMD) protein-DNA complex species, respectively (intermediary model). **ΔG MD2** is the dissociation free energy recovered in the simple association (two state model) fitting. **ΔG cooperative** was calculated using high cooperativity model in BIOEQS. **ΔGapp Bioeqs** was calculated as described in methodology from global analysis with BIOEQS, and **ΔGapp Hill** was calculated from Hill analysis.