2006, Volume 110B

Kaori Fukuzawa,* Yuji Mochizuki, Shigenori Tanaka, Kazuo Kitaura, and Tatsuya Nakano: Molecular Interactions between Estrogen Receptor and Its Ligand Studied by the ab Initio Fragment Molecular Orbital Method

The numerical results compiled in our published paper have slightly been changed by improving an inconsistency of the frozen-core setting in monomer and dimer treatments of the FMO-MP2 calculations. The corrected results, however, have not affected our qualitative discussions.

In Table 2, the MP2 energies are corrected, and the discussions in the original paper referring to the numerical values of Table 2 should be superseded by those of the corrected table. Corrections for Figure 4, which are very minor, are available in the Supporting Information. Because the total IFIEs between the ligand and all residues of ER are corrected to −96.1 and −101.1 kcal/mol at the MP2/6-31G and 6-31G* levels, respectively, the statement in the original paper concerning the energy difference (30 kcal/mol) between these two levels should be replaced by the following statement (p 16107):

> The energies at the MP2/6-31G and 6-31G* levels were similar. The addition of the polarization function slightly affected the interaction with hydrophobic residues.

Atomic charges and electron densities calculated at the MP2 level are also corrected (Figure 6). The numerical values in the original paper should be corrected after eq 3 (p 16108) as follows:

> The Δq for Glu353 indicated a large positive value, 0.122 e, and that for EST indicated a similar negative value, −0.109 e. Those for Arg394 and His524 also indicated small negative values, −0.024 e and −0.017 e, respectively. The Δq for Thr347 was smaller, 0.010 e, and this residue was therefore thought to have a lesser contribution to the CT interaction.

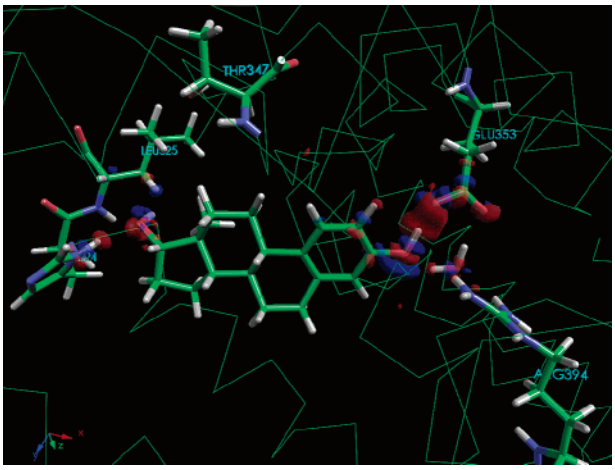

Figure 6. The difference in electron densities ($\Delta\rho$) between complexed and individual component molecules; $\Delta\rho = \rho$(complex) − (ρ(ER) + ρ(ligand)) calculated at the MP2/6-31G* level. The stick representation refers to EST, a water molecule, and residues (Glu353, Thr347, Arg394, His524, and Leu525) with significant $\Delta\rho$ values. The line representation is the C_α backbone. The red (minus) and blue (plus) represent the sign of the isosurfaces at ±0.002 e/bohr^3.

The overall discussions about the results and conclusions of the original paper are not affected.

Supporting Information Available: Figure 4 including numerical corrections for the MP2 energies. This material is available free of charge via the Internet at http://pubs.acs.org.

TABLE 2: IFIEs between EST and each amino acid residue of the ER[a]

method	HF								MP2			
basis set	STO-3G		6-31G		6-31G*		6-31G**		6-31G		6-31G*	
attractive interactions	Glu353	−39.28	Glu353	−27.92	Glu353	−27.75	Glu353	−28.19	Glu353	−29.59	Glu353	−32.23
	His524	−5.98	Arg394	−8.75	Arg394	−7.10	Arg394	−7.00	Arg394	−10.48	Arg394	−9.11
	Arg394	−5.27	Thr347	−5.41	Thr347	−5.04	Thr347	−4.87	His524	−8.74	His524	−8.80
	Thr347	−1.92	His524	−5.26	His524	−3.89	His524	−3.61	Thr347	−8.11	Thr347	−7.98
	Water	−1.02	**Met522**	**−2.44**	**Met522**	**−2.21**	**Met522**	**−2.19**	**Phe404**	**−4.46**	**Phe404**	**−5.12**
	Glu330	−0.92	**Met343**	**−1.85**	**Met343**	**−1.58**	**Met343**	**−1.57**	**Met343**	**−3.66**	**Leu387**	**−3.71**
	Met522	**−0.82**	Water	−1.59	Glu330	−1.20	Glu330	−1.17	**Leu346**	**−3.59**	**Leu346**	**−3.60**
	Lys531	−0.74	Glu330	−1.27	Lys531	−0.92	Lys531	−0.87	**Met522**	**−3.29**	**Met343**	**−3.55**
	Asp351	−0.71	Lys531	−1.02	**Met528**	**−0.91**	**Met528**	**−0.83**	**Ala350**	**−3.07**	**Met522**	**−3.32**
	Val392	**−0.66**	**Met528**	**−1.02**	**Gly344**	**−0.84**	**Gly344**	**−0.79**	**Leu387**	**−3.04**	**Ala350**	**−3.28**
	Ala350	**−0.64**	**Gly344**	**−1.00**	**Val392**	**−0.78**	**Val392**	**−0.74**	Water	−2.90	**Met388**	**−2.52**
	Glu542	−0.51	**Val392**	**−0.89**	Asp538	−0.74	Asp538	−0.73	**Leu384**	**−2.00**	Water	−2.48
	Ala405	**−0.49**	Asp538	−0.77	Glu542	−0.69	Glu542	−0.68	**Met421**	**−1.94**	**Leu384**	**−2.12**
	Asp538	−0.47	**Ala350**	**−0.74**	**Ala350**	**−0.66**	**Ala350**	**−0.62**	**Met388**	**−1.75**	**Met421**	**−2.04**
	Glu380	−0.45	Glu542	−0.72	Arg412	−0.62	Arg412	−0.61	Glu330	−1.27	**Leu391**	**−1.63**
	Arg412	−0.44	**Leu346**	**−0.72**	**Leu346**	**−0.61**	Arg436	−0.60	**Leu391**	**−1.18**	**Ile424**	**−1.29**
	Lys529	−0.38	Glu380	−0.67	Glu380	−0.61	Glu380	−0.60	**Ile424**	**−1.17**	Glu330	−1.20
	Gly344	**−0.38**	Arg436	−0.62	Arg436	−0.60	Asp351	−0.57	**Met528**	**−1.16**	**Met528**	**−1.13**
repulsive interactions	Arg352	1.83	**Leu391**	**1.79**	**Leu391**	**1.68**	**Leu391**	**1.70**	**Leu354**	0.96	Glu423	0.90
	Leu391	**2.35**	Arg352	2.69	**Met388**	**2.38**	**Met388**	**2.35**	Glu419	1.00	Glu419	0.95
	Met388	**2.51**	**Met388**	**2.76**	Arg352	2.52	Arg352	2.43	Glu339	1.25	Glu339	1.11
	Leu525	**5.15**	**Leu525**	**4.64**	**Leu525**	**4.41**	**Leu525**	**4.53**	Arg352	2.69	Arg352	2.52
[b]charged/polarized	−54.48		−50.42		−45.42		−45.11		−62.66		−63.31	
[c]**hydrophobic**	**12.02**		**4.95**		**5.15**		**5.77**		**−33.46**		**−37.77**	
[d]total	−42.46		−45.48		−40.26		−39.34		−96.13		−101.07	

[a] Only selected values with stronger interactions are shown, and they are listed in order of the interaction energy values. Hydrophobic residues are indicated as bold characters. Energies are in kcal/mol. [b] Sum of all IFIEs between EST and each charged or polarized residue in the ER. [c] Sum of all IFIEs between EST and each hydrophobic residue in the ER. [d] Sum of all IFIEs between EST and each residue in the ER.

10.1021/jp065705n CCC: $33.50
Published on Web 11/08/2006