

Residue-Specific pK_a Determination of Lysine and Arginine Side Chains by Indirect ¹⁵N and ¹³C NMR Spectroscopy: Application to *apo* Calmodulin [*J. Am. Chem. Soc.* **2007**, *129*, 15805–15813]. Ingemar André, Sara Linse, and Frans A. A. Mulder*

Page 15807. A typographical mistake was found in eq 1. The correct form of the Henderson-Hasselbalch equation for deprotonation should read

$$\delta_{\text{obs}} = \frac{(\delta_{\text{HA}} + \delta_{\text{A}^{-}} 10^{(\text{pH} - pK_a)})}{(1 + 10^{(\text{pH} - pK_a)})} \tag{1}$$

where δ_{obs} is the observed chemical shift and δ_{HA} and δ_{A^-} are the chemical shifts of the protonated and unprotonated forms, respectively.

Importantly, all data were analyzed with this correct form of eq 1, and in no way does this correction change the results or conclusions presented in the original paper. We thank Mr. Jelle Slager for bringing this mistake to our attention.

JA902385J

10.1021/ja902385j Published on Web 04/21/2009

Ligand Controlled Highly Regio- and Enantioselective Synthesis of α -Acyloxyketones by Palladium-Catalyzed Allylic Alkylation of 1,2-Enediol Carbonates [*J. Am. Chem. Soc.* 2008, *130*, 11852–11853]. Barry M. Trost,* Jiayi Xu, and Thomas Schmidt

Page 11853. In Table 2, entries 11 and 12, the stereochemical assignments of the cyclohexenyl ring of compound **20** and the cycloheptenyl ring of compound **22** should be *S*, not *R*. This assignment is based on the empirical model we proposed (Trost, B. M.; Toste, F. D. *J. Am. Chem. Soc.* **1999**, *121*, 4545), which has been supported by extensive experimental data.

JA902816Z

10.1021/ja902816z Published on Web 04/21/2009 Enantioselective Intramolecular Friedel-Crafts-Type α-Arylation of Aldehydes [*J. Am. Chem. Soc.* 2009, 131, 2086–2087]. K. C. Nicolaou,* Rüdiger Reingruber, David Sarlah, and Stefan Bräse

Page 2086. The intermediate in eq 1 should be a cation radical as follows:

The structures 1b and A in Table 1 should be as follows:

The intramolecular attack from the aromatic nucleus occurs from the Re face of the enamine when using (2R,5R)-A.

Page 2087. The structures of the products in Table 2, entries 3 and 10, should be as follows:

Correspondingly, Scheme 1 should be corrected as follows:

We deeply regret these oversights and errors. A corrected Supporting Information file that reflects these changes is available. These corrections have no implications on the main discoveries and conclusions described in the paper.

Supporting Information Available: Experimental procedures and compound characterization (corrected). This material is available free of charge via the Internet at http://pubs.acs.org.

JA902682T

10.1021/ja902682t Published on Web 04/15/2009 Valence Anions of 9-Methylguanine-1-Methylcytosine Complexes. Computational and Photoelectron Spectroscopy Studies [J. Am. Chem. Soc. 2009, 131, 2663-26691. Anna Szyperska, Janusz Rak,* Jerzy Leszczynski,* Xiang Li, Yeon Jae Ko, Haopeng Wang, and Kit H. Bowen*

Page 2668. In the last paragraph of section 3.2.2, the activation barrier for the proton transfer process from the N1 atom of methylguanine to the N3 atom of methylcytosine should be corrected as written below:

The kinetic barrier that separates a1MGMC and a1MGMC SPT2 structures is 2.78 and 2.39 kcal/mol in terms of energy and free energy, respectively.

The conclusion remains the same.

Page 2663–2664. An important reference was inadvertently omitted from the Introduction. Schaefer and co-workers¹ used the B3LYP/DZP++ theoretical approach to study the 2'deoxyguanosine-2'-deoxycytidine (dG:dC) nucleoside pair. Their research revealed that electron attachment to the dC moiety in the dG:dC pair is able to trigger proton transfer from N1(dG) to N3(dC), forming the more stable anionic complex d(G-H)⁻: d(C+H), and the energy barrier for this reaction is 2.4 kcal/ mol, which is in good agreement with data presented in our article.

Literature Cited

(1) Gu, J.; Xie, Y.; Schaefer, H. F., III J. Chem. Phys. 2007, 127, 155107/1-155107/6.

JA9020638

10.1021/ja9020638 Published on Web 04/20/2009 Jacobsen's Catalyst for Hydrolytic Kinetic Resolution: Structure Elucidation of Paramagnetic Co(III) Salen Complexes in Solution via Combined NMR and Quantum Chemical Studies [J. Am. Chem. Soc. 2009, 131, 4172-4173]. Sebastian Kemper, Peter Hrobárik, Martin Kaupp,* and Nils E. Schlörer*

Page 4173. Footnote a of Scheme 2 should read "S-epoxide" instead of "R-epoxide".

JA902706F

10.1021/ja902706f Published on Web 04/20/2009