Computational calculations in microwave-assisted organic synthesis (MAOS). Application to cycloaddition reactions

A. de Cózar, M. C. Millán, C. Cebrián, P. Prieto, A. Díaz-Ortiz, A. de la Hoz and F. P. Cossío

Org. Biomol. Chem., 2010, 8, 1000-1009 (DOI: 10.1039/b922730j)

The authors regret the following errors:

In Scheme 2 the structures of compounds 11 and 12 were incorrect. A corrected scheme is shown below.

Organocatalytic Michael addition of unprotected 3-substituted oxindoles to nitroolefins

Miao Ding, Feng Zhou, Zi-Qing Qian and Jian Zhou

Org. Biomol. Chem., 2010, 8, 2912–2914 (DOI: 10.1039/c004037a)

The authors regret the following errors:

- 1) The first row of Table 2, "R11" should be corrected to "R1".
- 2) In entry 14 of Table 2, the R should be "Bn", instead of "Ph", because 3-benzyloxindole was used in this case.

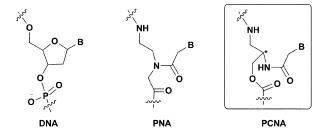
Design, synthesis and DNA/RNA binding studies of nucleic acids comprising stereoregular and acyclic polycarbamate backbone: polycarbamate nucleic acids (PCNA)

Vangala Madhuri and Vaijayanti A. Kumar

Org. Biomol. Chem., 2010, 8, 3734-3741 (DOI: 10.1039/c003405n)

The authors regret the following error:

In Fig. 1 a nitrogen atom was accidently omitted from the structure of PNA. The correct version of this figure is shown below.



Calix[4]pyrrole-based anion transporters with tuneable transport properties

Masafumi Yano, Christine C. Tong, Mark E. Light, Franz P. Schmidtchen and Philip A. Gale

Org. Biomol. Chem., 2010, 8, 4356–4363 (DOI: 10.1039/c0ob00128g)

In Table 2 the errors quoted for K_{ass} and ΔH^{o} are incorrect. The correct values are given below.

Table 2 Thermodynamic state functions of the 1:1 complexation of tetraalkylammonium salts by triazolo-calixpyrrole 3 as measured by ITC in acetonitrile at 303 K.

| entry | salt | $K_{\rm ass}$ / ${f M}^{-1}$ | $\Delta G^{\circ}/\mathrm{kcal}\ \mathrm{mol}^{-1}$ | $\Delta H^{\circ}/\mathrm{kcal}\ \mathrm{mol}^{-1}$ | $T\Delta S^{ m o}/{ m kcal~mol^{-1}}$ |
|-------|--|------------------------------|---|---|---------------------------------------|
| 410 | TEA chloride ^a | $2.6 \pm 0.26 \times 10^6$ | -8.89 | -11.88 ± 0.05 | -2.9 |
| 5 | TEA chloride ^b | $1.3 \pm 0.15 \times 10^6$ | -8.47 | -12.0 ± 0.05 | -3.5 |
| 6 | TEA benzoate ^b | $6.0 \pm 0.07 \times 10^3$ | -5.23 | -9.90 ± 0.05 | -4.7 |
| 7 | TBA | $1.3 \pm 0.04 \times 10^{3}$ | -4.32 | -8.54 ± 0.12 | -4.2 |
| | p-nitrobenzoate ^a | | | | |
| 8 | TBA acetate ^a | $1.6 \pm 0.16 \times 10^{5}$ | -7.23 | -13.1 ± 0.1 | -5.9 |
| 9 | TBA fluoride .3H ₂ O ^a | $1.5 \pm 0.20 \times 10^{5}$ | -7.19 | -11.3 ± 0.2 | -4.1 |
| 10 | TEA isocyanate ^b | $1.1 \pm 0.01 \times 10^6$ | -8.38 | -13.3 ± 0.04 | -4.9 |
| 11 | TBA H₂PO₄-b | $7.8 \pm 0.08 \times 10^{3}$ | -5.39 | -5.14 ± 0.01 | +0.2 |
| 12 | TEA hydrogencarbonate ^b | $2.0 \pm 0.10 \times 10^{5}$ | -7.36 | -11.4 ± 0.06 | -4.0 |

Efficient conversion of triacylglycerols and fatty acids to biodiesel in a microwave reactor using metal triflate catalysts

Aaron M. Socha and Jason K. Sello

Org. Biomol. Chem., 2010, 8, 4753-4756 (DOI: 10.1039/c0ob00014k)

The authors regret the following error:

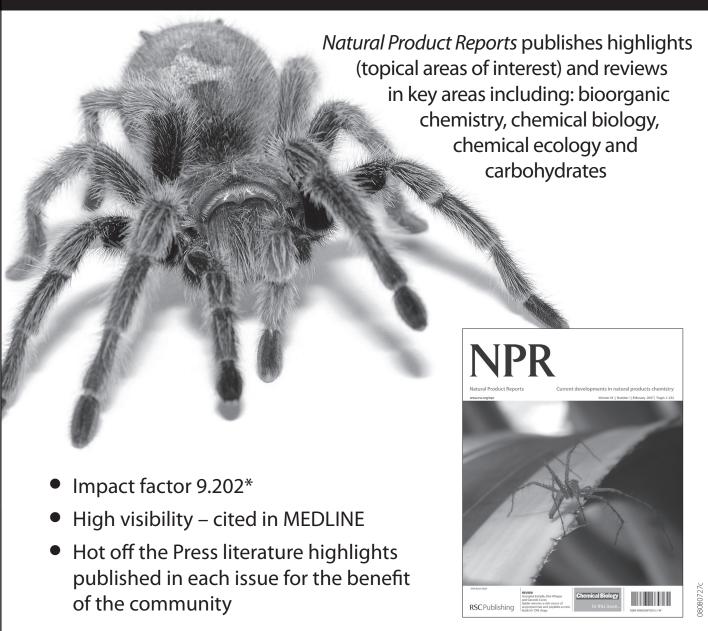
In Table 1, the headers for columns 4 and 5 (indicating reaction temperature and time) were mislabelled. The correct table is shown below:

| TAG | Catalyst ^a | MeOH eq. | Time (min) | T(°C) | Percent yield ^b |
|-----------|-----------------------|----------|------------|--------|----------------------------|
| | Cularyst | meerreq. | i mie (mm) | 1 (0) | r ereeme grena |
| Oleate | Sc(OTf)3 | 6 | 20 | 150 | 18 |
| Oleate | Sc(OTf) ₃ | 12 | 20 | 150 | 31 |
| Oleate | Sc(OTf) ₃ | 48 | 20 | 150 | 92 |
| Oleate | Bi(OTf) ₃ | 48 | 25 | 150 | 85 |
| Linoleate | Sc(OTf) ₃ | 48 | 20 | 150 | 90 |
| Linoleate | Bi(OTf) ₃ | 48 | 25 | 150 | 84 |
| Myristate | Sc(OTf) ₃ | 48 | 30 | 150 | 82 |
| Myristate | Bi(OTf) ₃ | 48 | 25 | 150 | 99 |
| Palmitate | Sc(OTf) ₃ | 48 | 20 | 150 | 99 |
| Palmitate | Bi(OTf) ₃ | 48 | 25 | 150 | 92 |

[&]quot;10 mol % catalyst loading bYields calculated by GC-MS15,16

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers. Additions and corrections can be viewed online by accessing the original article to which they apply.

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