

the equation  $y = 1/(1 + x/b)$ , where  $x$  is the inhibitor concentration,  $y$  is the relative activity, and  $b$  is the  $IC_{50}$  value. The concentrations of stock solutions of **1** were calculated from  $A_{262}$  measurements using  $\epsilon = 9890 \text{ M}^{-1} \text{ cm}^{-1}$ .

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## Additions and Corrections

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Yu Liu,\* Yi-Min Zhang, Ai-Di Qi, Rong-Ti Chen, Keiko Yamamoto, Takehiko Wada, and Yoshihisa Inoue\*. Molecular Recognition Study on a Supramolecular System. 10. Inclusion Complexation of Modified  $\beta$ -Cyclodextrins with Amino Acids: Enhanced Enantioselectivity for L/D-Leucine.

Page 1827. After publishing the paper, we found that mono[6-(*m*-toluidinyl)-6-deoxy]- $\beta$ -cyclodextrin (**1**) was contaminated by the starting material, mono[6-*O*-(*p*-toluenesulfonyl)]- $\beta$ -cyclodextrin, probably due to the insufficient reaction period and the subsequent incomplete purification. As for the  $^1\text{H}$  NMR data reported, the signals observed at  $\delta$  7.41–7.44 and 7.73–7.75, which had been erroneously assigned to the aromatic protons of **1**, should be assigned to those of the starting material, mono[6-*O*-(*p*-toluenesulfonyl)]- $\beta$ -cyclodextrin. From the integrated area of the original spectrum, we found that the “toluidinyl-CD” prepared previously contained *ca.* 40–50% of the starting material.

We therefore prepared a pure sample of compound **1** again and determined the binding constants for the enantiomeric pairs of the same amino acids. The revised synthetic procedure described below is similar to that reported earlier, except for the extended reaction period and the isolation procedure. The enantioselectivities calculated from the corrected binding constants have turned out to be considerably smaller than the previous values.

**Mono[6-(*m*-toluidinyl)-6-deoxy]- $\beta$ -cyclodextrin** was prepared by the reaction of mono[6-*O*-(*p*-toluenesulfonyl)]- $\beta$ -cyclodextrin with *m*-toluidine (10 mL) in *N,N*-dimethylformamide (20 mL) at 85 °C with stirring for 3 days under  $\text{N}_2$ . The reaction mixture was evaporated in vacuo at 40 °C to dryness. The residue was dissolved in water, and acetone was added to the resulting solution to give a gray precipitate. After drying, the product was purified by chromatography over Sephadex to give the pure sample of **1** in 50% yield. MS: *m/e* 1246 (calcd for  $(\text{M} + \text{Na} - \text{H})$  1246). IR (KBr)/ $\text{cm}^{-1}$ : 3364, 2909, 1716, 1625, 1542, 1412, 1361, 1338, 1307, 1233, 1147, 1071, 1018, 933, 841, 749, 695, 573, 518.  $^1\text{H}$  NMR (DMSO-*d*<sub>6</sub>, TMS, ppm):  $\delta$  2.1 (s, 3H,  $\text{CH}_3$ ), 3.1–3.8 (m, 42H), 4.3–4.6 (m, 6H), 4.6–4.9 (m, 7H), 5.0–5.2 (m, 1 H, NH), 5.6–5.9 (m, 14H), 6.2–6.4 (m, 3H, Ar-H), 6.8–6.9 (t, 1H, Ar-H). Anal. Calcd for  $\text{C}_{49}\text{O}_{34}\text{H}_{77}\text{N}\cdot 5\text{H}_2\text{O}$ : C, 44.78; H, 6.67; N, 1.07. Found: C, 44.63; H, 6.75; N, 1.01.

We further repeated the complexation experiment with the pure host **1** prepared above to determine the complex stability constants ( $K_s$ ), according to the reported procedure. The data obtained are listed in Table 1A.

As can be seen from Table 1A, the stability constants, especially the enantioselectivities, are significantly dif-

ferent from the previous data. One reasonable explanation is that the compound reported previously contained a considerable amount of mono[6-*O*-(*p*-toluenesulfonyl)]- $\beta$ -cyclodextrin, which is not fluorescent at all but yet influences the inclusion complexation. Another possible reason would be that there are some technical problems inherently in the Benesi–Hildebrand method, so the constants obtained in that way should be taken with some reservations (Szejtli, J. *Cyclodextrins and Their Inclusion Complexes*; Akademiai Kiado: Budapest (Hungary), 1982; p 199).

**Supporting Information Available:**  $^1\text{H}$  NMR spectra for compounds **4–9** and **1** (7 pages). This material is contained in libraries on microfiche, immediately follows this article in the microfilm version of the journal, and can be ordered from the ACS; see any current masthead page for ordering information.

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**Table 1A. Complex Stability Constant ( $K_s$ ) and Gibbs Free Energy Change ( $-\Delta G$ ) for the Supramolecular System Formed by 6-(*m*-Toluidinyl)-6-deoxy- $\beta$ -cyclodextrin (**1**) and Some Aliphatic Amino Acids<sup>a</sup>**

host	guest	$K_s$	$\log K_s$	$-\Delta G$ (kJ/mol)	$-\Delta\Delta G$ (kJ/mol)
6-( <i>m</i> -toluidinyl)-6-deoxy- $\beta$ -cyclodextrin	L-Ala	1197	3.08	17.3	0.4
	D-Ala	1430	3.16	17.7	
	L-Ser	843	2.93	16.4	1.3
	D-Ser	1406	3.15	17.7	
	L-Val	416	2.62	14.7	0.9
	D-Val	609	2.78	15.6	
	L-Leu	1439	3.16	17.7	-0.9
	D-Leu	1002	3.00	16.8	

<sup>a</sup> Measured in a phosphate buffer (pH 7.20) at room temperature (20–23 °C).

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**Lin-Hua Zhang,\* Goss S. Kauffman, Jaan A. Pesti, and Jianguo Yin.** Rearrangement of  $\text{N}_\alpha$ -Protected L-Asparagine with Iodosobenzene Diacetate. A Practical Route to  $\beta$ -Amino-L-alanine Derivatives.

Page 6919, Table 1. Compounds **3** and **4** mentioned in this table have been previously prepared by Dr. R. Pascal et al. using 1,1-diacetoxyiodobenzene in DMF (Mendre, C.; Pascal, R.; Calas, B. *Tetrahedron Lett.* **1994**, 35, 5429–5432. Sola, R.; Sagner, P.; David, M.-L.; Pascal, R. *Chem. Commun.* **1993**, 1786–1788). We thank Dr. Pascal for bringing this to our attention.

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