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Correction

Correction: Monaco et al. Chiral Phase Transfer Catalysis in the Asymmetric Synthesis of a 3,3-Disubstituted Isoindolinone and Determination of Its Absolute Configuration by VCD Spectroscopy. *Molecules* 2020, *25*, 2272

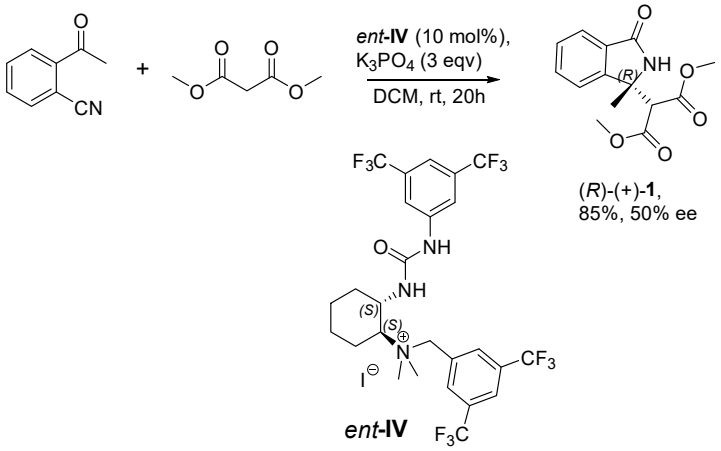
Guglielmo Monaco [1,*], Maximilian Tiffner [2], Antonia Di Mola [1], Wouter Herrebout [3], Mario Waser [2] and Antonio Massa [1,*]

[1] Dipartimento di Chimica e Biologia, Università di Salerno, Via Giovanni Paolo II, 132, 84084 Fisciano, SA, Italy
[2] Institute of Organic Chemistry, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria
[3] Department of Chemistry, University of Antwerp, B-2020 Antwerp, Belgium
* Correspondence: gmonaco@unisa.it (G.M.); amassa@unisa.it (A.M.); Tel.: +39-089969570 (G.M.); +39-089969565 (A.M.)

In this note, we report a correction to the published article, *Molecules* **2020**, *25*, 2272; doi:10.3390/molecules25102272 [1], regarding the absolute configuration (AC) of the used catalyst **IV** in the preparation of the sample sent for a VCD analysis.

In the paper, the VCD analysis was performed on the sample (+)-**1** to determine its absolute configuration and it was found that the AC is (*R*). This new compound was in fact synthetized with the catalyst (*S*,*S*)-**IV** (*ent*-**IV** in the article), while in the text it was erroneously reported that the used catalyst was **IV** with the (*R*,*R*) configuration.

Therefore, the reaction scheme should be corrected as follows:



Scheme 1. Asymmetric cascade reaction of 2-acetylbenzonitrile with dimethylmalonate.

Some other parts of the article must be corrected, as on page 4:

Under the best conditions of entry 1 of Table 3, the reaction was scaled up to 100 mg of 2-acetylbenzonitrile, using catalyst *ent*-**IV** (with *S*,*S* configuration), obtaining similar results in terms of yield and ee (90% and 50%, respectively). The enantiopurity of the product was further improved by means of a heterochiral crystallization process (**1** crystallizes as a racemate), leading to the isolation of **1** from the mother liquor in up to 96% ee and in an acceptable efficiency (45% yield), thus resulting in an overall process (asymmetric catalytic cyclization followed by crystallization) allowing for considerable quantities of almost enantiopure isoindolinone **1** from simple starting materials. This sample was used for the determination of the Absolute Configuration by VCD.

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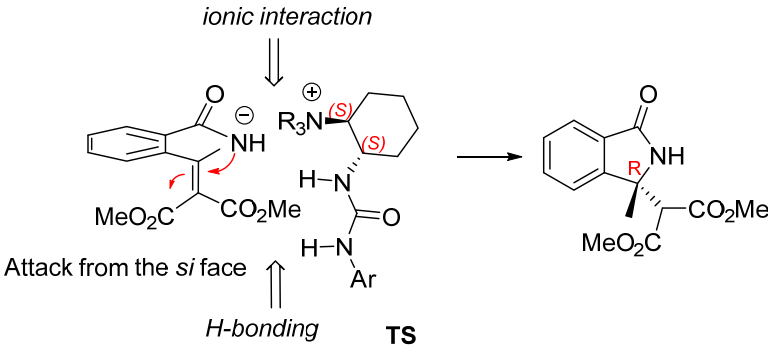
In addition, the proposed reported mechanism of Scheme 2 [1] must be revised considering different interactions in the TS, as follows:



Scheme 2. Proposed transition state.

The nature of this exact interaction mode remains speculative, but it is obvious that the bifunctional nature of the catalyst is crucial for obtaining the promising enantioselectivities achieved herein (the *S*,*S*-catalyst gives mainly the *R* product; the configuration is determined as described in the following chapter).

The experimental section, in particular:

3.2. Procedure of Asymmetric Synthesis and Crystallization of **1**

In a typical procedure, a mixture of 2-acetylbenzonitrile (14 mg, 0.1 mmol) in CH2Cl2 (1.8 mL), catalyst **IV** (5 mol%), anhydrous K3PO4 (64 mg, 3 eqv.), and dimethylmalonate (34 µL, 3 eqv.) was stirred at room temperature until the disappearance of the starting material (TLC, Hexane/Ethyl acetate, 4:6). The solution was filtered and purified on silica gel (Hexane/Ethyl acetate, 70:30 to 50:50) obtaining a white solid. Yield: 85% (23.5 mg, 0.085 mmol). The spectroscopic data are in accordance with the literature [12]. Ee: 50%, Chiralpak IA3, Hex/IPA 80:20, 0.6 mL/min, λ: 254 nm, t: 17.52 min and 20.90 min. The reaction was also scaled up to 100 mg of 2-acetylbenzonitrile with cat. *ent*-**IV** with an (*S*,*S*) configuration (0.714 mmol) giving similar results in terms of yield and ee of the opposite enantiomer. Procedure for crystallization of **1a**. A sample of 40 mg, obtained from the above scale-up procedure, was dissolved in a mixture of CHCl3 (500 µL) and hexane (1.00 mL) at room temperature and then left at −20 °C for 72 h. The enantio-enriched product was recovered by filtration and evaporation of the solution, yielding 18 mg of (*R*)-**1** with 96% ee. $[\alpha]^{20}D$: +104.0 (c 0.80, $CHCl_3$). This sample was then used in VCD analysis.

The authors state that the scientific conclusions are unaffected. The original publication has also been updated.

Reference

1. Monaco, G.; Tiffner, M.; Di Mola, A.; Herrebout, W.; Waser, M.; Massa, A. Chiral phase transfer catalysis in the asymmetric synthesis of a 3,3-disubstituted isoindolinone and determination of its absolute configuration by VCD Spectroscopy. *Molecules* **2020**, *25*, 2272. [CrossRef] [PubMed]