

Corrections to Discovery of Leukotriene A4 Hydrolase Inhibitors Using Metabolomics Biased Fragment Crystallography [*J. Med. Chem.* 2009, 52, 4694. DOI: 10.1021/jm900259h]. Douglas R. Davies, Bjorn Mamat, Olafur T. Magnusson, Jeff Christensen, Magnus H. Haraldsson, Rama Mishra, Brian Pease, Erik Hansen, Jasbir Singh, David Zembower, Hidong Kim, Alex S. Kiselyov, Alex B. Burgin, Mark E. Gurney, and Lance J. Stewart*

Page 4702. In Figure 2, the chemical structure of compound **19** (DG-051) was incorrectly drawn as the (*R*)-enantiomer. Compound **19** is the (*S*)-enantiomer and is properly shown in the three-dimensional crystal structure image at the right-hand side in the corrected figure below.

On page 4704, right hand column, first paragraph, line 19 and second paragraph line 22, (*R*)-prolinol should be changed to (*S*)-prolinol.

Supporting Information Page S16. In Table 2, the chemical structure of compound **19** (DG-051) was incorrectly drawn as the (*R*)-enantiomer. The correct (*S*)-enantiomer has been included in the revised version of Supplemental Table 2 below.

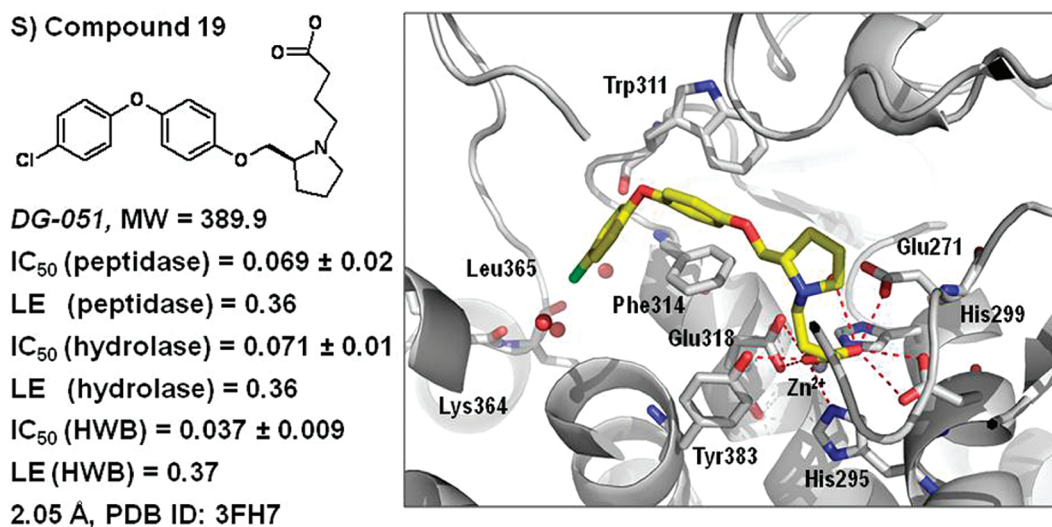
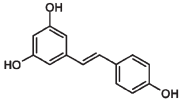
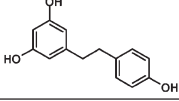
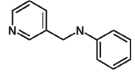
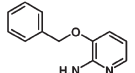
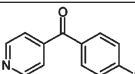
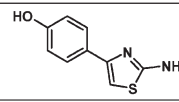
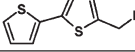
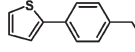
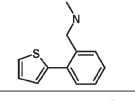
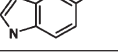
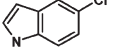
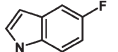
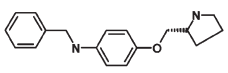
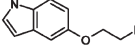
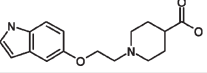
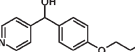
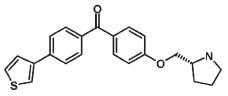
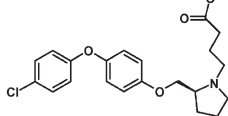


Figure 2. Panels showing ligand binding to LTA4H for compounds described in the manuscript. Enzyme assay IC_{50} values are in μ M, human whole blood cell assay IC_{50} values are in nM when reported, and ligand efficiency (LE) values are in kcal/(mol·heavy atom). Compound structures are displayed as yellow stick structures, and LTA4H is displayed in gray. Green mesh corresponds to the $F_o - F_c$ (difference) electron density at the 3.0σ level of the crystal structure with the compound omitted from the model. Polar contacts with LTA4H and/or bound water molecules are shown as red dashed lines. PDB IDs for each structure are indicated.

Supplemental Table 2. Comparative IC₅₀ data for peptidase, hydrolase, and HWB assays.

| Compound | Structure | Hydrolase Assay IC ₅₀ (μM) Mean ± SEM (N) | Peptidase Assay IC ₅₀ (μM) Mean ± SEM (N) | Human Whole Blood Assay IC ₅₀ (μM) Mean ± SEM (N) |
|----------------|---|--|--|--|
| 2 |  | 212 ± 40 (N=3) | 366 ± 67 (N=3) | n/d |
| 3 |  | 247 ± 26 (N=3) | 145 ± 26 (N=3) | n/d |
| 4 |  | 1667 ± 168 (N=2) | 1321 ± 257 (N=3) | n/d |
| 5 |  | 619 ± 131 (N=3) | 308 ± 39 (N=4) | n/d |
| 6 |  | 5308 (N=1) | 3673 ± 153 (N=3) | n/d |
| 7 |  | 1443 ± 63 (N=2) | >1000 (N=3) | n/d |
| 8 |  | 75.2 ± 7.3 (N=4) | 38.9 ± 15.9 (N=4) | n/d |
| 9 |  | 106 ± 20 (N=3) | 106 ± 23 (N=4) | n/d |
| 10 |  | >2000 (N=1) | 1077 ± 59 (N=4) | n/d |
| 11 |  | >2000 (N=1) | >1000 (N=3) | n/d |
| 12 |  | 1510 ± 139 (N=3) | >1000 (N=1) | n/d |
| 13 |  | >2000 (N=3) | >1000 (N=1) | n/d |
| 14 |  | 0.157 ± 0.032 (N=4) | 0.207 ± 0.053 (N=4) | 0.131 ± 0.057 (N=3) |
| 15 |  | 234 ± 21 (N=3) | 321 ± 44 (N=4) | n/d |
| 16 |  | 966 ± 322 (N=3) | 1491 ± 291 (N=3) | n/d |
| 17 |  | 170 ± 5 (N=3) | 202 ± 17 (N=3) | n/d |
| 18 |  | 0.189 ± 0.017 (N=3) | 0.0805±0.0185 (N=4) | 4.58 ± 1.33 (N=2) |
| 19 (DG-051) |  | 0.0708 ± 0.0140 (N=4) | 0.0685±0.0161 (N=4) | 0.0373 ± 0.0094 (N=9) |

Supplemental Table 2. Comparative IC₅₀ data for peptidase, hydrolase, and HWB assays. For all compound structures described in this work, inhibition assays were carried out using at least two independent methods, either the hydrolase assay, peptidase assay and/or a hydrolase assay in human whole blood. See Materials and Methods section for details. All results are given as IC₅₀ values in μM, with the number of replicates and the standard error of the mean indicated where applicable.