

Supporting Information
for
**Artificial Diels–Alderase based on the
transmembrane protein FhuA**

Hassan Osseili^{‡,1}, Daniel F. Sauer^{‡,1}, Klaus Beckerle¹, Marcus Arlt², Tomoki
Himiyama³, Tino Polen⁴, Akira Onoda³, Ulrich Schwaneberg², Takashi Hayashi³ and
Jun Okuda^{*,1}

Address: ¹Institute of Inorganic Chemistry, RWTH Aachen University, Landoltweg 1,
52056 Aachen, Germany, ²Institute of Biotechnology, RWTH Aachen University,
Worringer Weg 1, 52056 Aachen, Germany, ³Department of Applied Chemistry,
Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita 565-0871,
Japan and ⁴Institute of Bio- and Geosciences IBG-1: Biotechnology,
Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

Email: Jun Okuda - jun.okuda@ac.rwth-aachen.de

*Corresponding author

[‡]Equal contributors

**Illustration of the catalyst 2 and NMR spectra of synthesized
compounds**

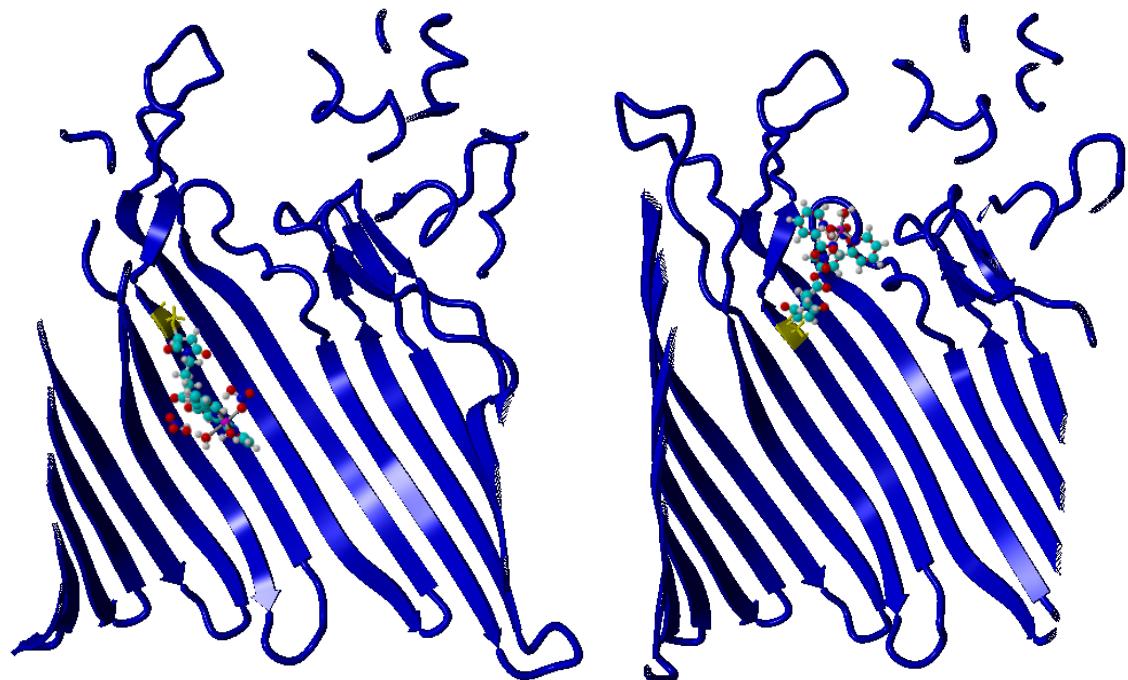


Figure S1: Illustration of the catalyst **2** within the cavity of FhuA.

NMR spectra of synthesized compounds

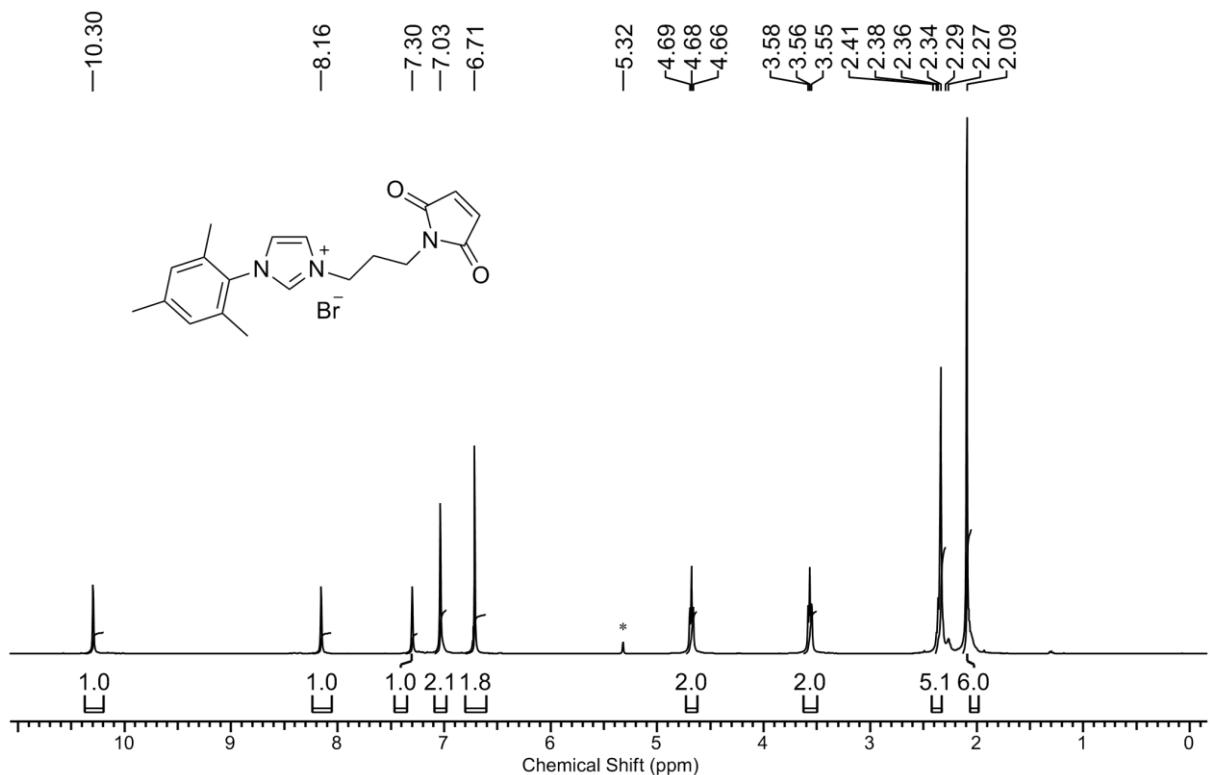


Figure S2. ^1H NMR spectrum (23 °C, $^3\text{CD}_2\text{Cl}_2$) of compound 3.

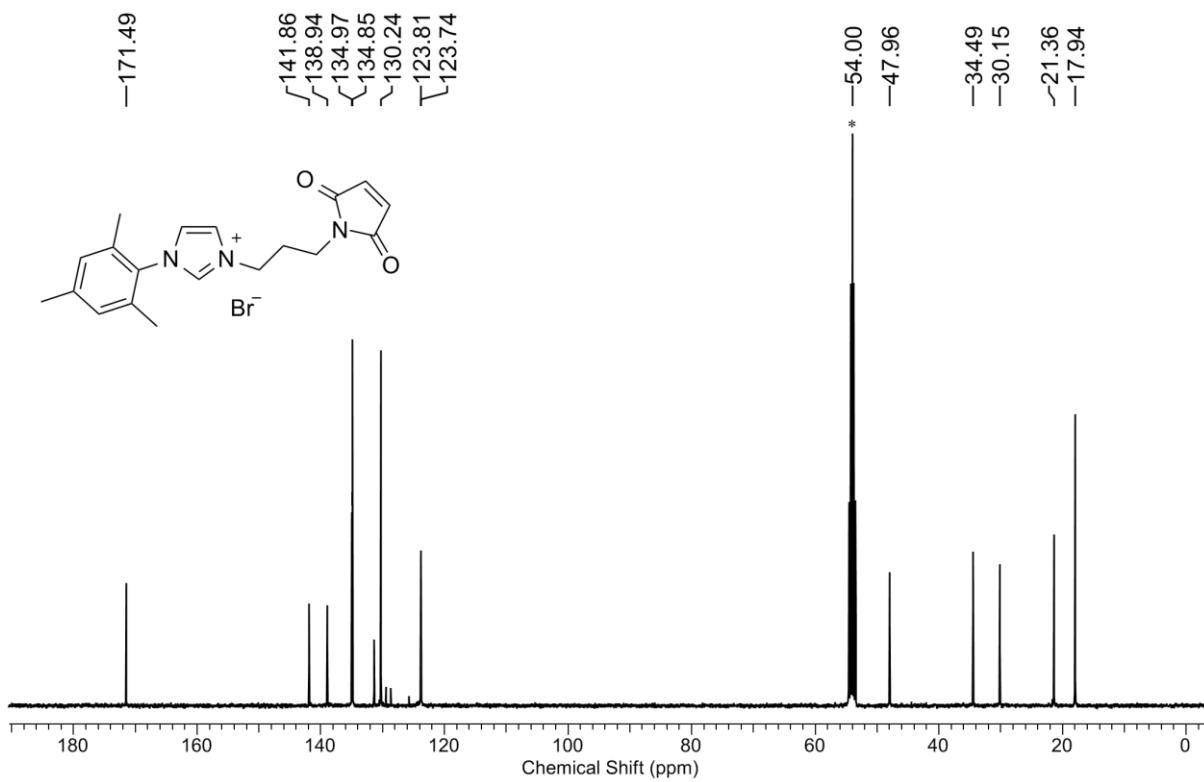


Figure S3. ^{13}C NMR spectrum (23 °C, $^{\text{3}}\text{CD}_2\text{Cl}_2$) of compound 3.

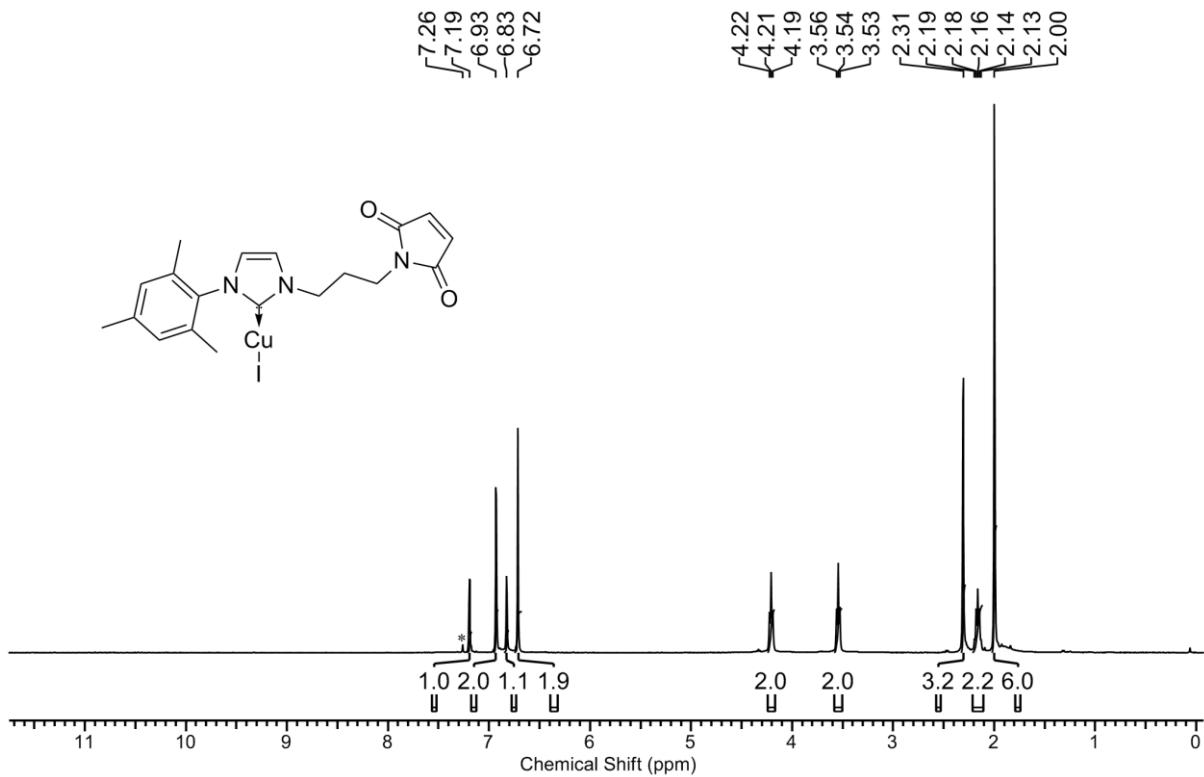


Figure S4. ^1H NMR spectrum (23 °C, $^6\text{CDCl}_3$) of compound 4.

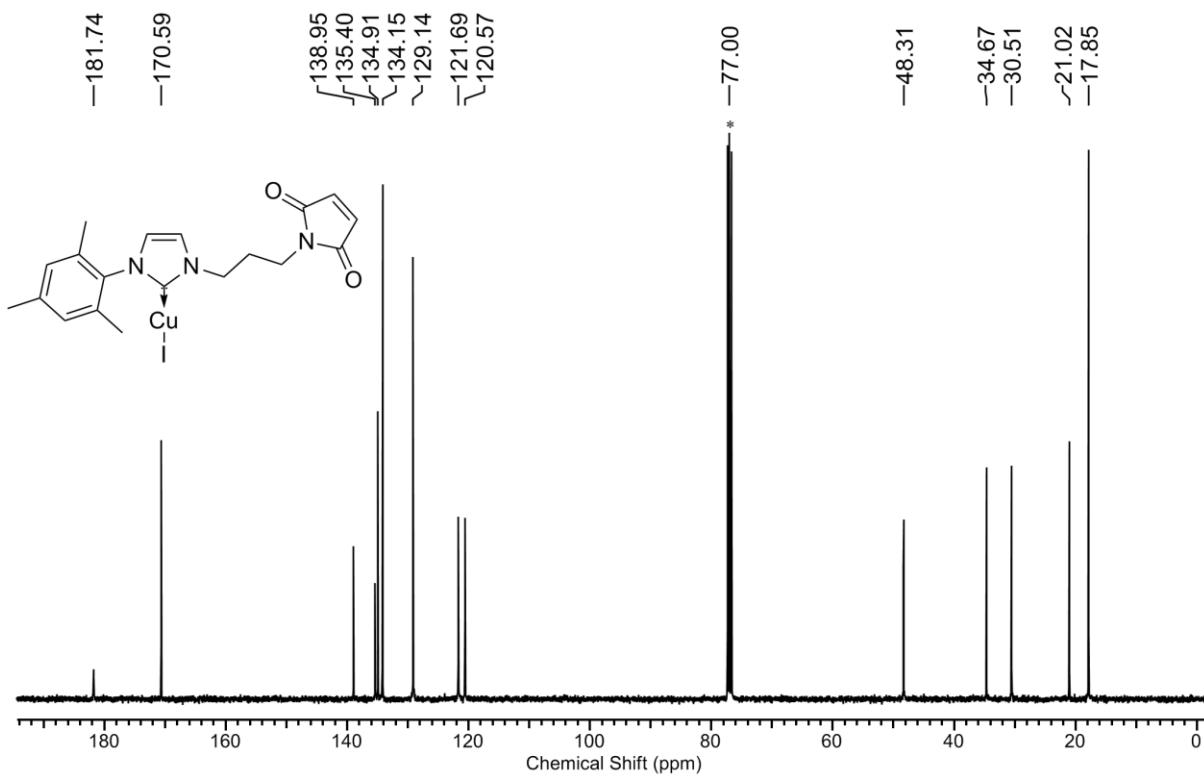


Figure S5. ^{13}C NMR spectrum (23 °C, ${}^*\text{CDCl}_3$) of compound 4.

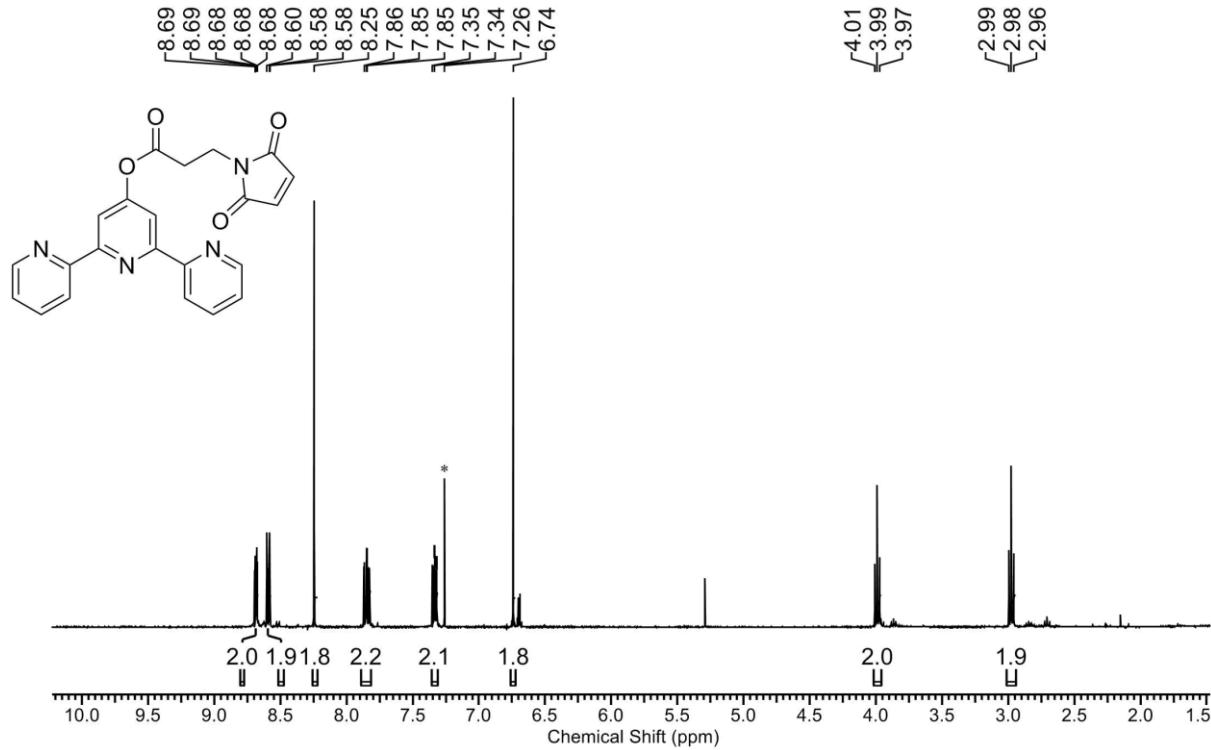


Figure S6. ^1H NMR spectrum (23 °C, ${}^*\text{CDCl}_3$) of compound 8.

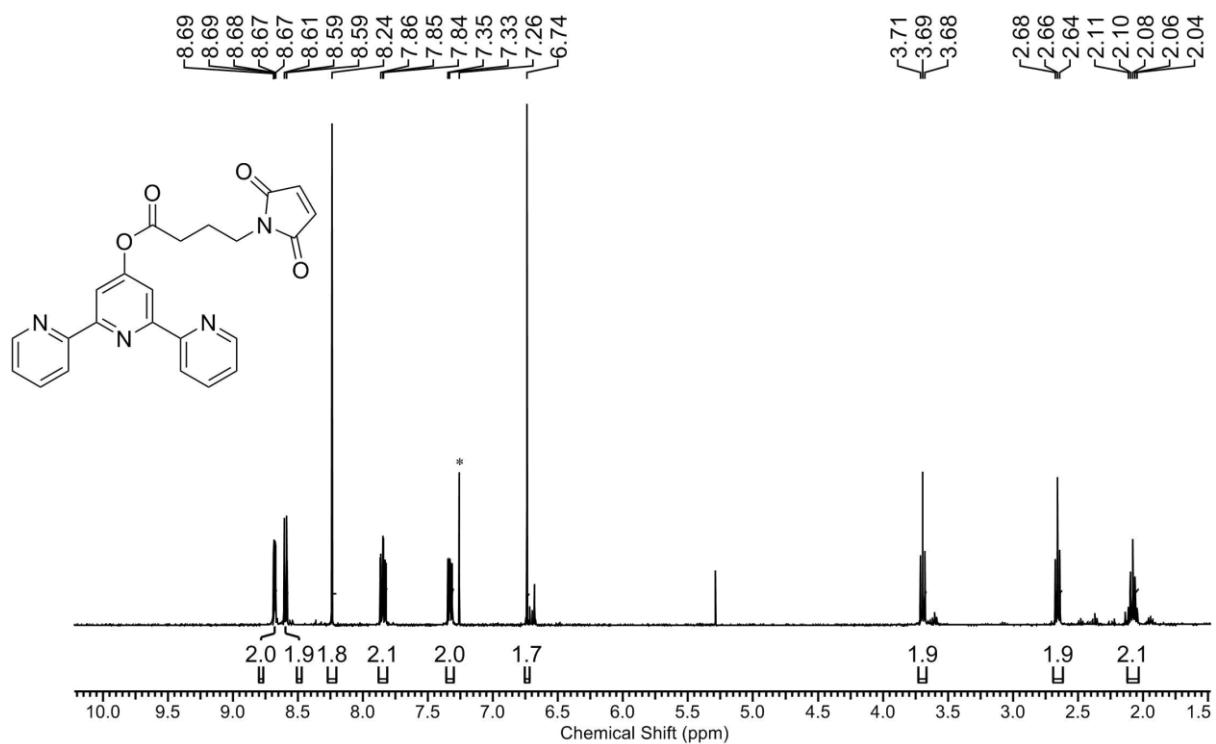


Figure S7. ¹H NMR spectrum (23 °C, ³CDCl₃) of compound **9**.