Supporting information

Enzymatic Kinetic Resolution of Chiral Sulfoxides - An Enantiocomplementary Approach

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1. General

All starting reagents were commercially available and of analytical purity, which were used without further treatment unless otherwise stated. Racemic sulfoxides were prepared according to the literature procedures\textsuperscript{1–4} unless otherwise stated. Solvents were dried according to standard methods. \(^1\)H NMR spectra were obtained at 400 MHz. \(^{13}\)C NMR spectra were obtained at 100 MHz and were \(^1\)H decoupled. Chemical shifts (\(\delta\)) are reported in ppm relative to solvent ((CH\(_3\))\(_2\)SO: \(\delta_C = 40.2\) ppm) or residual solvent peak ((CH\(_3\))\(_2\)SO: \(\delta_H = 2.50\) ppm). Accurate mass measurements (HRMS) were obtained by ESI on an Agilent 6530 Q-TOF MS spectrometer. Analytical HPLC was performed under the following conditions: Agilent Eclipse plus C18 column (3.5 \(\mu\)L, 4.6\(\times\)100 mm); UV/Vis detection at \(\lambda_{obs} = 254\) nm, 220 nm or 300 nm; flow rate 0.4 mL/min; gradient elution method (0.1% aqueous formic acid – CH\(_3\)CN from 95:5 to 0:100 in 13 min. Analytical TLC was performed using a precoated silica gel 60 Å F\(_{254}\) plates (0.2 mm thickness) and visualized by irradiation with UV light at 254 nm or by dipping in stain solution (KMnO\(_4\), CAM) followed by heating. Preparative column chromatography was carried out using silica gel 60 Å (particle size 0.063–0.200 mm). Enantiomeric excesses were determined by chiral HPLC analysis using Daicel Chiralpak (IA, IC) and Chiralcel OD-H columns and a mixture of \(n\)-heptane/propan-2-ol as the eluent. The detailed conditions are given at the characterization part of the products. The absolute configurations of the products were determined by the comparison of chiral HPLC retention times and optical rotation values with the literature. Selectivity factor \(s\) was calculated according to formula \(s = \ln[(1-c)(1-ee)]/\ln[(1-c)(1+ee)]\).\textsuperscript{5} Optical rotations were measured on an automatic polarimeter Autopol III. Infrared spectra were recorded on a Thermo Nicolet Avatar 370 FT-IR spectrophotometer. Purifications by HPLC were performed under the following conditions: Agilent ZORBAX SBC18 column (5 \(\mu\)L, 9.4\(\times\)150 mm); UV/Vis detection at \(\lambda_{obs} = 254\) and 300 nm; flow rate 4 mL/min; gradient elution methods (method 0.1% ammonium formate in H\(_2\)O – CH\(_3\)CN from 50:50 to 0:100 in 20 min.
2. Preparation of Methionine Sulfoxide Reductases B (H. sapiens (CBS-1), N. gonorrhoeae (pilB), T. kodakarensis (MsrB) and A. thaliana (MsrB2))

Genes of MsrB domains (H. sapiens (CBS-1), N. gonorrhoeae (pilB), T. kodakarensis (MsrB)) in pET16b vectors from Genescript and MsrB2 (A. thaliana) in pQE30 vector were transformed into chemically competent E. coli BL21(DE3) cells (Agilent) according to the manufacturer's protocol and an aliquot was plated on LB agar with ampicillin (100 mg/L) and grew overnight at 37 °C. One colony of E. coli BL21(DE3) with the corresponding MsrB was used for overnight preculture, then the preculture (0.4 mL) was used to inoculate 100 ml of LB medium with ampicillin (100 mg/L). The bacterial culture was incubated at 37 °C, 200 rpm until OD$_{600}$ ~ 0.4 was reached. Then the production of MsrB was induced either with 0.2 mM IPTG (MsrB2 from A. thaliana) or 0.5 mM IPTG (all other MsrBs) and the culture was incubated either at 22 °C (MsrB2 from A. thaliana) or at 37 °C (all other MsrBs), 200 rpm overnight. Cells were harvested by centrifugation (4000 × g for 30 min at 4 °C). The cell pellet was resuspended in LEW buffer (50 mM NaH$_2$PO$_4$, 300 mM NaCl, pH 8) and lysed by ultrasound. Cell debris was removed by centrifugation (10 000 × g for 30 min at 4 °C), the soluble fraction was loaded onto Protino Ni-IDA resin column (Macherey-Nagel) and purified by gravity flow at ambient temperature. The column was washed with 2 × 8 mL of LEW buffer and finally the protein was eluted with 2 × 2 mL of elution buffer (50 mM NaH$_2$PO$_4$, 300 mM NaCl, 250 mM imidazole, pH 8). Purity was determined via SDS-PAGE. Elution buffer was exchanged to storage buffer (20 mM Tris-HCl buffer, 1 mM DTT, 10% glycerol, 0.1 M NaCl, pH 8.0) with Amicon Ultra-4 centrifugal filter (3000 MWCO) and yielded approximately 10 mg of protein. Purification of CBS-1 reductase provided only a very low yield of the desired product and thus this reductase was not used in further experiments. Protein concentration was determined from the absorbance at 280 nm (using calculated extinction coefficient).

Fig. S1: (a) SDS-PAGE MsrB2 (A. thaliana): (M)-protein mass marker, (1)-lysate, (2)-flow through, (3)-elution; (b): SDS-PAGE MsrBs: (M)-protein mass marker; CBS-1 (H. sapiens): (1)-lysate, (2)- flow through, (3)- elution; PilB (N. gonorrhoeae): (4)-lysate, (5)- flow through, (6)- elution; MsrB (T. kodakarensis): (7)-lysate, (8)- flow through, (9)- elution.
3. Procedure for the Kinetic Resolution of Racemic Sulfoxides with Isolated Enzymes MsrBs (*N. gonorrhoeae* (pilB), *T. kodakarensis* (MsrB) and *A. thaliana* (MsrB2))

A 1.5 mL Eppendorf vial was charged with individual solutions of DTT (1440 µL of 27 mM, 4 equivs., 26 mM final concentration) in phosphate buffer (50 mM Na$_2$HPO$_4$, 50 mM NaH$_2$PO$_4$, 50 mM NaCl, pH 7.5) and a racemic sulfoxide (30 µL of 324 mM, 9.7 µmol, 6.5 mM final concentration) in CH$_3$CN. The resulting mixture was gently mixed and the reaction was initiated by the addition of the corresponding MsrB (1 mol%, 65 µM final concentration) in a storage buffer. The reaction mixture was incubated at 37 °C at 250 rpm. The course of the reaction was monitored by analytical HPLC. After 44 h the reaction with the highest conversion of 44% (MsrB2 *A. thaliana*) was selected for further analysis (the conversion of the reactions with the other MsrBs was below 10%). The reaction mixture was extracted with toluene (2 × 4 mL), washed with H$_2$O (2 mL), brine (2 mL), dried under MgSO$_4$ and concentrated by rotary evaporation under reduced pressure. The enantiomeric excess of the crude product was determined by chiral HPLC (ee = 63%) providing $s = 17$. 

![Diagram of reaction](image-url)
4. General Procedure for the Kinetic Resolution of Racemic Sulfoxides with DmsABC reductase

\[ \text{rac-S} \rightarrow \text{(S)-1} + \text{2} \]

A 2 mL preculture of *E. coli* (msrA knock out - KEIO collection ID JW4178)\(^{10}\) was used to inoculate 400 mL LB medium with kanamycin (50 mg/L). The bacterial culture was incubated at 37 °C, 200 rpm until OD\(_{600}\) of 3 was reached. Then, 47 mL aliquot of the bacterial culture was withdrawn, and cells were harvested by centrifugation (4200 × g, 30 min, 4 °C). The cell pellet was washed with M9 minimal medium (48 mM Na\(_2\)HPO\(_4\), 22 mM KH\(_2\)PO\(_4\), 8.6 mM NaCl, 18.7 mM NH\(_4\)Cl, 2 mM MgSO\(_4\), 0.1 mM CaCl\(_2\), 0.4% glycerol, pH 7.0) and centrifuged (4200 × g, 30 min, 4 °C). Cells resuspended in M9 minimal medium (2 mL) were added to a mixture of racemic sulfoxide (0.065 mmol) in M9 minimal medium (8 mL) in 100mL Erlenmeyer flask and then decane (0.5 mL) was added. The final OD\(_{600}\) in the reaction mixture was 14 (0.2 ppm of DmsABC) unless otherwise stated. The reaction mixture was incubated at 37 °C, 200 rpm. The conversion of the reaction was determined by analytical HPLC. Then, the reaction mixture was centrifuged (16900 × g, 2 min, 4 °C). The supernatant was extracted with EtOAc (4 ml), the organic phase was washed with H\(_2\)O (1 mL) and brine (1 ml), dried over MgSO\(_4\), and concentrated by rotary evaporation under reduced pressure. The enantiomeric excess was determined by chiral HPLC. The absolute configuration of the sulfoxides was determined by comparison of the HPLC retention times and the optical rotation with the reported data.\(^1\)

A modified protocol was utilized for substrates 1n-1p. Due to low solubility and acidic instability of the substrates,\(^1\) pH of M9 minimal buffer was adjusted to 9.0 and methanol (2 %) was added to the reaction. Decane as co-solvent was omitted in these experiments. Also, reactions were carried out at 14.5 μmol scale.

\((S)-1\)-Methyl-4-(methylsulfinyl)benzene (1a)\(^1\)

![Structure of (S)-1-Methyl-4-(methylsulfinyl)benzene (1a)](structure.png)

C\(_8\)H\(_{10}\)OS (154.23 g/mol), conversion 50% in 2 h, \(s > 100\). The enantiomeric excess (ee > 99%) was determined by HPLC (ODH chiralcel: heptane/propan-2-ol (98:2); flow rate 1mL/min; 25 °C; 254 nm; \(t_{R} = 32.1\) and 35.7 min).
(S)-1-Methyl-3-(methylsulfinyl)benzene (1b)

C₈H₁₀OS (154.23 g/mol), conversion 50% in 1 h, s > 100. The enantiomeric excess (ee > 99%) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1mL/min; 25 °C; 254 nm; tᵣ = 24.4 and 29.9 min).

(S)-1-Methyl-2-(methylsulfinyl)benzene (1c)

C₈H₁₀OS (154.23 g/mol), final OD₆₀₀ = 28 (0.4 ppm of DmsABC), conversion 50% in 2 h, s > 100. The enantiomeric excess (ee = 98%) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1mL/min; 25 °C, 254 nm, tᵣ = 23.2 and 24.8 min).

(S)-1-(Ethylsulfinyl)-4-methylbenzene (1d)

C₉H₁₂OS (168.25 g/mol), final OD₆₀₀ = 28 (0.4 ppm of DmsABC), conversion 52% in 2 h, s > 100. The enantiomeric excess (ee = 99%) was determined by HPLC (IA chiralpak: heptane/propan-2-ol (95:5); flow rate 0.5 mL/min; 25 °C; 254 nm; tᵣ = 27.4 and 29.2 min).

(S)-1-(Propylsulfinyl)-4-methylbenzene (1e)

C₁₀H₁₄OS (182.28 g/mol), final OD₆₀₀ = 28 (0.4 ppm of DmsABC), conversion 39% in 2 h, s = 3. The enantiomeric excess (ee = 26%) was determined by HPLC (IA chiralpak: heptane/propan-2-ol (95:5); flow rate 1 mL/min; 25 °C; 254 nm; tᵣ = 12.9 and 13.7 min).

1-(Isopropylsulfinyl)-4-methylbenzene (1f)

C₁₀H₁₄OS (182.28 g/mol), final OD₆₀₀ = 28 (0.4 ppm of DmsABC), conversion 9% in 2 h, s = 0. The enantiomeric excess (ee = 0%) was determined by HPLC (IA chiralpak: heptane/propan-2-ol (95:5); flow rate 1 mL/min; 25 °C; 254 nm; tᵣ = 12.0 and 12.8 min).
(R)-1-((chloromethyl)sulfinyl)-4-methylbenzene (1g)²

C₈H₁₀ClOS (188.67 g/mol), final OD₆₀₀ = 28 (0.4 ppm of DmsABC), conversion 52 % in 2 h, s > 100. The enantiomeric excess (ee = 99 %) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1 mL/min; 25 °C; 254 nm; rₑ = 17.8.7 and 19.4 min). ; [α]²⁵_D = 139.0 (c = 0.5, CHCl₃), lit: +136 (c = 1.0, CHCl₃) for (S), ee = 95 %²

(S)-1-Bromo-4-(methylsulfinyl)benzene (1h)¹

C₇H₇BrOS (219.10 g/mol), conversion 51 % in 1 h, s > 100. The enantiomeric excess (ee > 99%) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1mL/min; 25 °C; 254 nm; rₑ = 18.6 and 20.2 min).

(S)-4-(Methylsulfinyl)benzonitrile (1i)¹

C₈H₇NOS (165.21 g/mol), conversion 52 % in 1 h, s > 100. The enantiomeric excess (ee = 99 %) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1mL/min; 25 °C; 254 nm; rₑ = 47.0 and 51.3 min).

(S)-1-Methoxy-4-(methylsulfinyl)benzene (1j)¹

C₈H₁₀O₂S (170.23 g/mol), conversion 48% in 1 h, s > 100. The enantiomeric excess (ee = 98%) was determined by HPLC (ODH chiralcel: heptane/propan-2-ol (90:10); flow rate 1mL/min; 25 °C; 254 nm; rₑ = 17.0 and 18.1 min).

(S)-((Methylsulfinyl)methyl)benzene (1k)¹

C₈H₁₀OS (154.23 g/mol), conversion 48% in 1 h, s > 100. The enantiomeric excess (ee = 99%) was determined by HPLC (IA chiralpak: heptane/propan-2-ol (95:5); flow rate 1mL/min; 25 °C; 25 °C; 220 nm; rₑ = 21.9 and 24.0 min).
(S)- ((Ethylsulfinyl)methyl)benzene (1l)\(^1\)

\[
\begin{align*}
\text{C}_9\text{H}_{12}\text{OS} & \quad (168.25 \text{ g/mol}), \ \text{conversion} \ 49\% \ \text{in} \ 1 \ \text{h}, \ s \ > \ 100. \ \text{The enantiomeric excess (ee = 99\%)} \ \text{was determined by HPLC (IC chiralpak: heptane/propan-2-ol (80:20); flow rate 1mL/min; 25 °C; 220 nm; } t_r = 24.0 \ \text{and 26.5 min).}
\end{align*}
\]

(S)- (2-(Methylsulfinyl)ethyl)benzene (1m)\(^1\)

\[
\begin{align*}
\text{C}_9\text{H}_{12}\text{OS} & \quad (168.25 \text{ g/mol}), \ \text{conversion} \ 51\% \ \text{in} \ 1 \ \text{h}, \ s \ > \ 100. \ \text{The enantiomeric excess (ee = 99\%)} \ \text{was determined by HPLC (IA chiralpak: heptane/propan-2-ol (95:5); 1mL/min; 25 °C; 220 nm; } t_r = 23.1 \ \text{and 25.2 min).}
\end{align*}
\]

Esomeprazole (1n)\(^{11}\)

\[
\begin{align*}
\text{C}_{17}\text{H}_{19}\text{N}_3\text{O}_3\text{S} & \quad (345.42 \text{ g/mol}), \ 14.5 \ \mu\text{mol scale}, \ \text{final OD}_{600} = 40 (2.0 \ \text{ppm of DmsABC}), \ \text{conversion} \ 29\% \ \text{in} \ 2 \ \text{h}, \ s \ > \ 100. \ \text{The enantiomeric excess (ee = 40\%)} \ \text{was determined by HPLC (IC chiralpak: heptane/propan-2-ol (60:40); 1mL/min; 25 °C; 300 nm; } t_r = 20.4 \ \text{and 33.3 min).}
\end{align*}
\]

5-methoxy-2-(propylsulfinyl)-1H-benzo[d]imidazole (1o)

\[
\begin{align*}
\text{C}_{11}\text{H}_{14}\text{N}_2\text{O}_2\text{S} & \quad (238.31 \text{ g/mol}), \ 14.5 \ \mu\text{mol scale}, \ \text{final OD}_{600} = 40 (2.0 \ \text{ppm of DmsABC}), \ \text{conversion} \ 42\% \ \text{in} \ 2 \ \text{h}, \ s = 3. \ \text{The enantiomeric excess (ee = 28\%)} \ \text{was determined by HPLC (IC chiralpak: heptane/propan-2-ol (60:40); 1mL/min; 25 °C; 300 nm; } t_r = 6.3 \ \text{and 7.7 min).}
\end{align*}
\]

2-((p-Tolylsulfinyl)methyl)pyridine (1p)\(^4\)

\[
\begin{align*}
\text{C}_{13}\text{H}_{13}\text{NOS} & \quad (231.31 \text{ g/mol}), \ 14.5 \ \mu\text{mol scale}, \ \text{final OD}_{600} = 40 (2.0 \ \text{ppm of DmsABC}), \ \text{conversion} \ 20\% \ \text{in} \ 2 \ \text{h}, \ s = 3. \ \text{The enantiomeric excess (ee = 11\%)} \ \text{was determined by HPLC (IC chiralpak: heptane/propan-2-ol (60:40); 1mL/min; 25 °C; 254 nm; } t_r = 21.5 \ \text{and 29.4 min).}
\end{align*}
\]

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\(^1\) 1.58.0

\(^{11}\) 2.1.58.0

\(^4\) 5.1.58.0
5. Proteomic Analysis

Cell pellets in 100 mM triethylammonium bicarbonate (TEAB) buffer containing 1% sodium deoxycholate (SDC) were boiled at 95°C for 5 min. Protein concentration was determined using BCA protein assay kit (Thermo) and 20 µg of protein per sample was used for MS sample preparation. Cysteines were reduced with 5 mM final concentration of tris(2-carboxyethyl)phosphine (TCEP) at 60 °C for 60 min, and blocked with 10 mM S-methyl methanethiosulfonate (MMTS) for 10 min at room temperature. Samples were digested with trypsin (trypsin/protein ratio of 1/20) at 37 °C overnight. After digestion samples were acidified with trifluoroacetic acid (TFA) to 1% final concentration. SDC was removed by extraction to ethylacetate and peptides were desalted on Michrom C18 column.14

Nano reversed phase column (EASY-Spray column, 50 cm × 75 µm ID, PepMap C18, 2 µm particles, 100 Å pore size) was used for LC/MS analysis. Mobile phase buffer A was composed of water and 0.1% formic acid. Mobile phase B was composed of acetonitrile and 0.1% formic acid. Samples were loaded onto the trap column (Acclaim PepMap300, C18, 5 µm, 300 Å Wide Pore, 300 µm × 5 mm) at a flow rate of 15 µL/min. Loading buffer was composed of water, 2% acetonitrile and 0.1% TFA. Peptides were eluted with gradient of B from 4% to 35% over 60 min at a flow rate of 300 nL/min. Eluting peptide cations were converted to gas-phase ions by electrospray ionization and analyzed on a Thermo Orbitrap Fusion (Q-OT- qIT, Thermo). Survey scans of peptide precursors from 400 to 1600 m/z were performed at 120K resolution (at 200 m/z) with a 5 × 10^5 ion count target. Tandem MS was performed by isolation at 1.5 Da with the quadrupole, HCD fragmentation with normalized collision energy of 30, and rapid scan MS analysis in the ion trap. The MS2 ion count target was set to 10^4, and the max injection time was 35 ms. Only those precursors with charge state 2–6 were sampled for MS2. The dynamic exclusion duration was set to 45 s with a 10 ppm tolerance around the selected precursor and its isotopes. Monoisotopic precursor selection was turned on. The instrument was run in top speed mode with 2 s cycles.

All data were analyzed and quantified with the MaxQuant software (version 1.5.3.8)15 The false discovery rate (FDR) was set to 1% for both proteins and peptides and we specified a minimum length of seven amino acids. The Andromeda search engine was used for the MS/MS spectra search against the Escherichia coli database (downloaded from Uniprot on November 2016, containing 6 072 entries). Enzyme specificity was set as C-terminal to Arg and Lys, also allowing cleavage at proline bonds and a maximum of two missed cleavages. Dithiomethylation of cysteine was selected as fixed modification and N-terminal protein acetylation and methionine oxidation as variable modifications. The “match between runs” feature of MaxQuant was used to transfer identifications to other LC-MS/MS runs based on their masses and retention times (maximum deviation 0.7 min) and this was also used in quantification experiments. Quantifications were performed with the label-free algorithms described recently.16 Data analysis was performed using Perseus 1.5.2.4 software.17
5. Procedure for Kinetic Resolution of Omeprazole

2.5 mL preculture of *E. coli* (msrA knock out - KEIO collection ID JW4178)\textsuperscript{10} was used to inoculate each of three 500 mL LB media with kanamycin (50 mg/L) in three 2 L Erlenmeyer flask. The bacterial cultures were incubated at 37 °C, 200 rpm until OD\textsubscript{600} of 3 was reached (6 hours). Then, cells were harvested by centrifugation (4200 × g, 30 min, 4 °C). Resuspended cells in M9 minimal medium (10 mL, pH 9) were added to a solution of racemic omeprazole (50 mg, 0.145 mmol, final concentration 0.5 mg/mL) in M9 minimal medium (88 mL, pH 9) and methanol (2 mL) in 1 L Erlenmeyer flask. The reaction mixture was incubated at 37 °C, 200 rpm in the dark. The conversion of the reaction was determined by analytical HPLC. After 3 h (conversion = 56 %), the reaction mixture was centrifuged (4200 × g, 20 min, 4 °C) and the supernatant was extracted with diethyl ether (4 × 200 mL), the organic phase was washed with H\textsubscript{2}O (40 mL) and brine (40 ml), dried over anhydrous MgSO\textsubscript{4} and concentrated by rotary evaporation under reduced pressure. Purification of the crude product by HPLC afforded \textbf{1n} in 36% yield (18 mg) as an off-white solid; [\(\alpha\r{25}^D\)] = –147° (c 0.2, CHCl\textsubscript{3}); lit: [\(\alpha\r{25}^D\)] = –157° (c 0.5, CHCl\textsubscript{3}) for (S)-omeprazole sodium salt, ee > 99%\textsuperscript{11}. Enantiomeric excess (ee = 98 %) was determined by HPLC (IC chiralpak: heptane/propan-2-ol (60:40); 1mL/min; 25 °C; 300 nm; \(t\r{r} = 18.1\) and 29.4 min).
6. Preparation of Racemic Sulfoxide 1o

*rac*-5-methoxy-2-(propylsulfinyl)-1H-benzo[d]imidazole (1o)

Compound 1o was prepared according to modified protocols\textsuperscript{19,20}.

To a solution of 5-methoxybenzimidazole-2-thiol (360 mg, 2 mmol) in ethanol (10 mL), water (2 mL) and sodium hydroxide (160 mg, 4 mmol), propyl 4-tolylsulfonate (419 mg, 2 mmol) was added portionwise and the reaction mixture was stirred first at room temperature for 2 h and then at 70 °C overnight. Then, reaction mixture was extracted with dichloromethane (3 × 40 mL) and the organic phase was washed with water (10 mL) and brine (20 mL), dried over anhydrous MgSO\textsubscript{4} and concentrated by rotary evaporation under reduced pressure to provide crude sulfide, which was used in the next step without further purification. To a stirred solution of a crude sulfide in dichloromethane (20 mL) and methanol (1 mL), solution of \textit{m}-chloroperoxybenzoic acid (≤77\%, 450 mg, 2 mmol) in dichloromethane (10 mL) was added dropwise and the reaction mixture was stirred at \textdegree C for 1 h. Reaction mixture was diluted with dichloromethane (70 mL), washed with saturated NaHCO\textsubscript{3} (20 mL), 10\% solution of NaS\textsubscript{2}O\textsubscript{3} (10 mL), water (10 mL) and brine (10 mL), dried over MgSO\textsubscript{4} and concentrated by rotary evaporation under reduced pressure. Purification of the crude product by column chromatography on silica gel (dichloromethane/methanol 10/1 then 5/1) afforded 1o in 47 \% yield (222 mg) as a viscous oil. \textit{\textsuperscript{1}H NMR} (400 MHz, (CD\textsubscript{3})\textsubscript{2}SO): 13.42 (bs, 1H), 7.53 (d, \textit{J} = 8.9 Hz, 1H), 7.08 (s, 1H), 6.91 (d, \textit{J} = 8.9 Hz, 1H), 3.80 (s, 3H), 3.26-3.13 (m, 2H), 1.80-1.67 (m, 1H), 1.60-1.47 (m, 1H), 0.98 (t, 3H). \textit{\textsuperscript{13}C NMR} (101 MHz, (CD\textsubscript{3})\textsubscript{2}SO): 156.9, 153.4, 137.4, 119.2, 113.7 (2 C), 97.8, 55.9, 55.6, 15.5, 13.3. \textit{HRMS (ESI)}: \textit{m/z} [M+H]\textsuperscript{+} calcd for C\textsubscript{11}H\textsubscript{15}N\textsubscript{2}O\textsubscript{2}S\textsuperscript{+} 239.0849; found: 239.0849. \textit{IR(KBr + acetone)}: 3070, 1625, 1413, 1305, 1272, 1204, 1156, 1024.
7. References

8. HPLC Traces: Kinetic Resolution with Isolated Enzyme MsrB (*A. thaliana*)

![HPLC Trace Image]

**Peak Table**

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9. HPLC Traces: Kinetic Resolution with DmsABC (whole E. coli cells)
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![Graph](image-url)
Peak Table

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<th>Area %</th>
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Peak Table

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### Peak Table

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### Peak Table

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10. HPLC Traces: Preparative Kinetic Resolution of Omeprazole

![Esomeprazole](image)

**Peak Table**

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**Peak Table**

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11. NMR Spectra
$^1$H NMR (400 MHz, (CD$_3$)$_2$SO) of rac-10
$^{13}$C NMR (101 MHz, (CD$_3$)$_2$SO) of 10