Supporting information

CIPROFLOXACIN-POLYMER CONJUGATES TARGETED WITH IRON(III) FOR EFFECTIVE TREATMENT OF INTRACELLULAR BACTERIAL INFECTIONS

Anna Stehlíková, Lenka Kotrchová, Michal Pechar, Kristýna Gunár, Eliška Rydvalová, Martin Studenovský, Tomáš Etrych*

Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, Prague 6, Czech Republic

*Corresponding author: etrych@imc.cas.cz, tel. +420-296809231

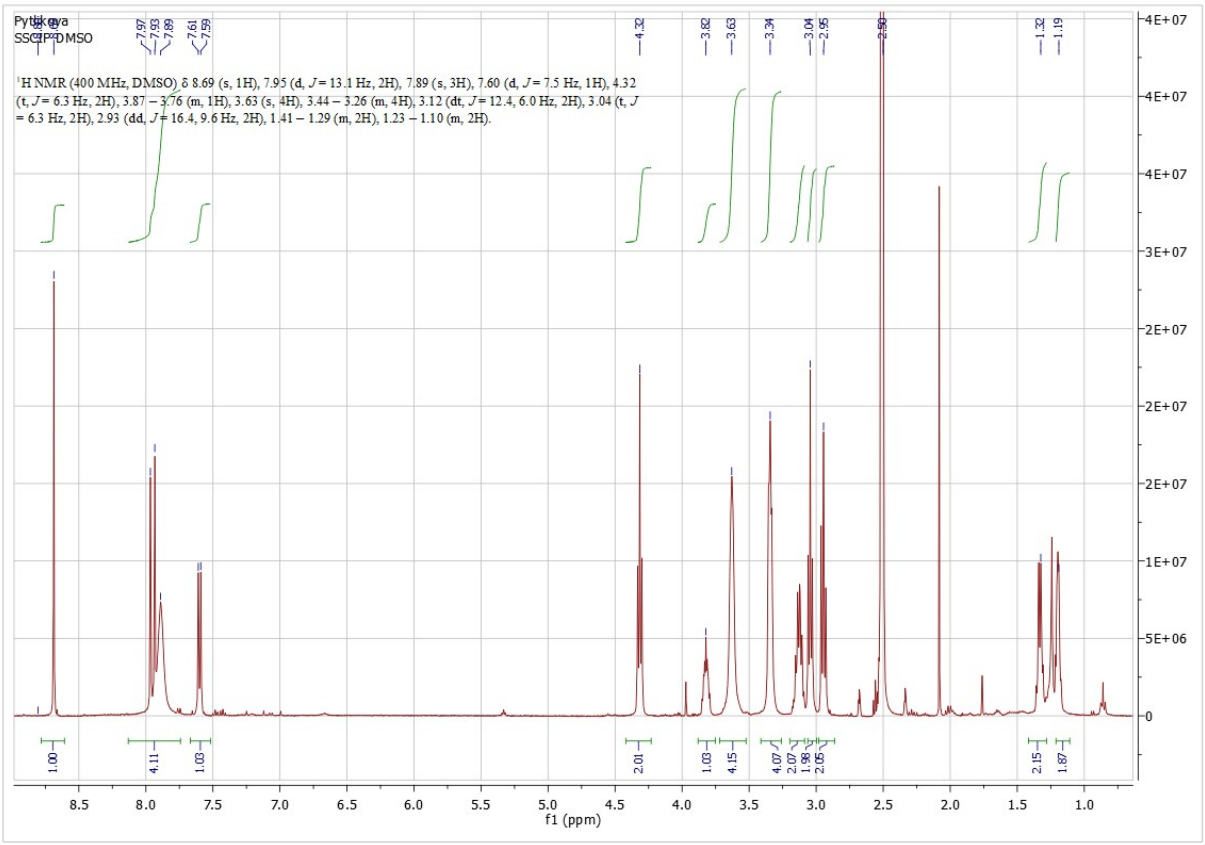

Figure S1 ^{1}H NMR spectrum of **SSCip** recorded in *d*6-DMSO at 400Mhz.

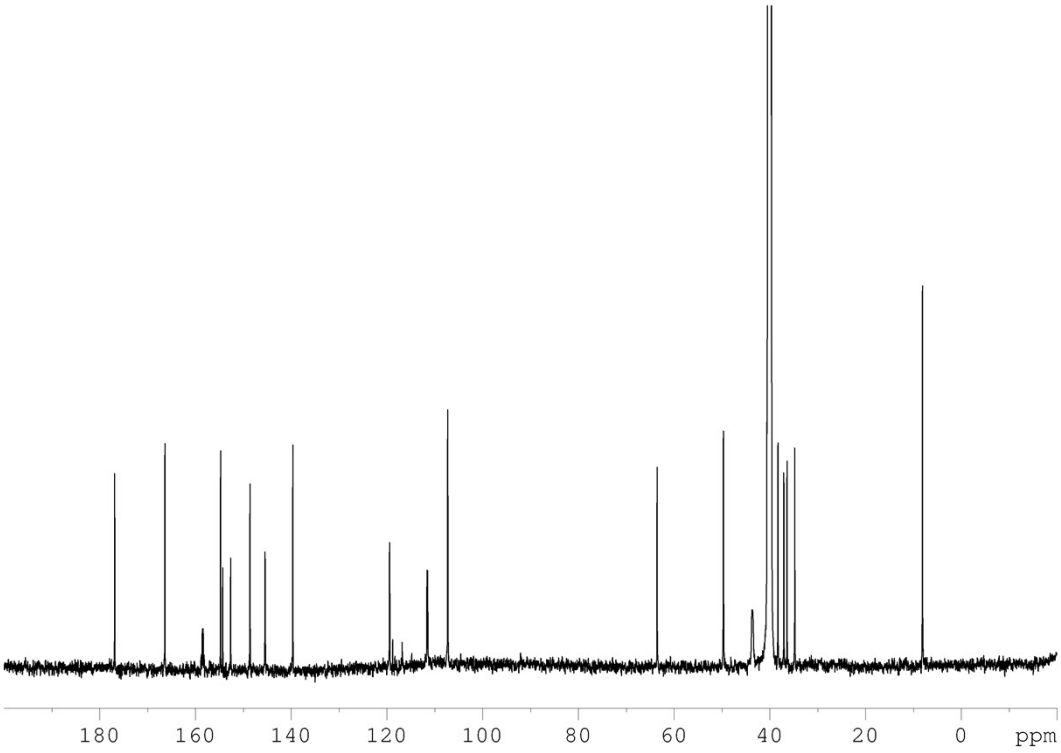

Figure S2 ^{13}C NMR spectrum of **SSCip** recorded in *d*6-DMSO at 600Mhz

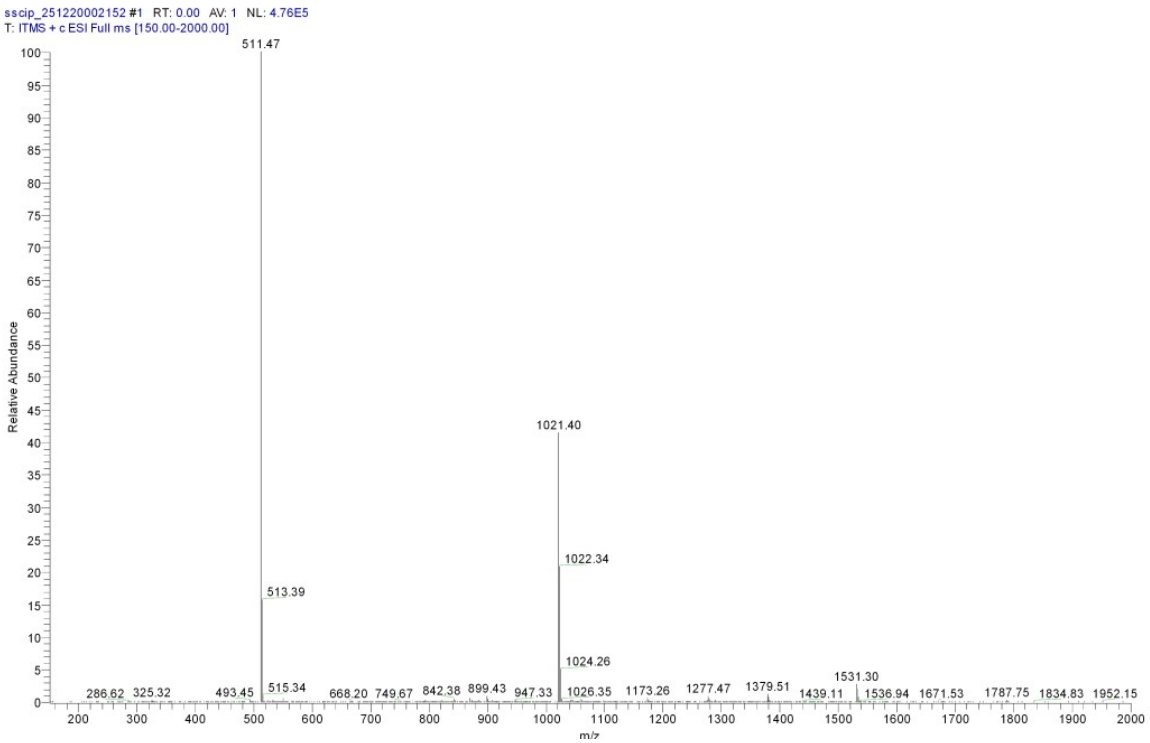

Figure S3 ESI–MS spectrum of SSCip recorded by electrospray ionization mass spectrometry (ESI–MS) using an LCQ Fleet mass analyzer (Thermo Fisher Scientific, Inc., Waltham, MA, USA).

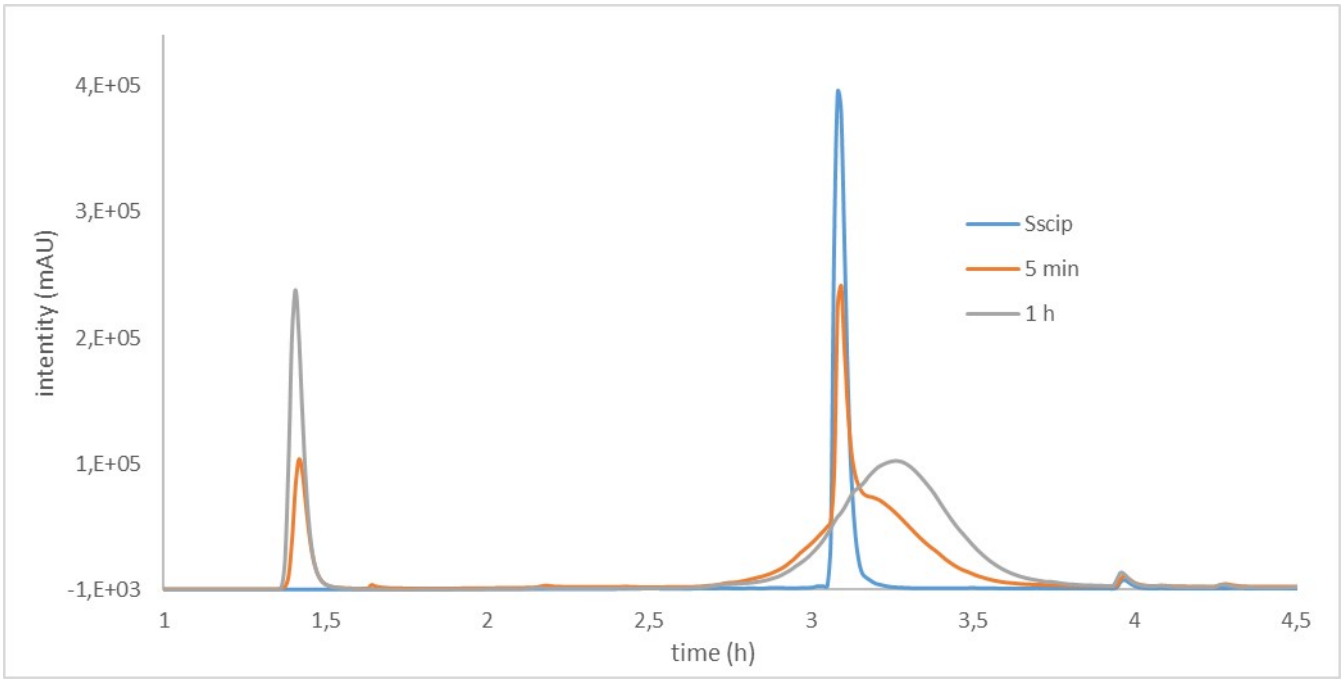

Figure S4 HPLC monitoring of the reaction between **SSCip** and the polymer precursor **P1** leading to the formation of the cleavable conjugate **PC**. Chromatograms were recorded at 280 nm on a Chromolith® C18 column using a TFA-containing mobile phase. The peak correspond

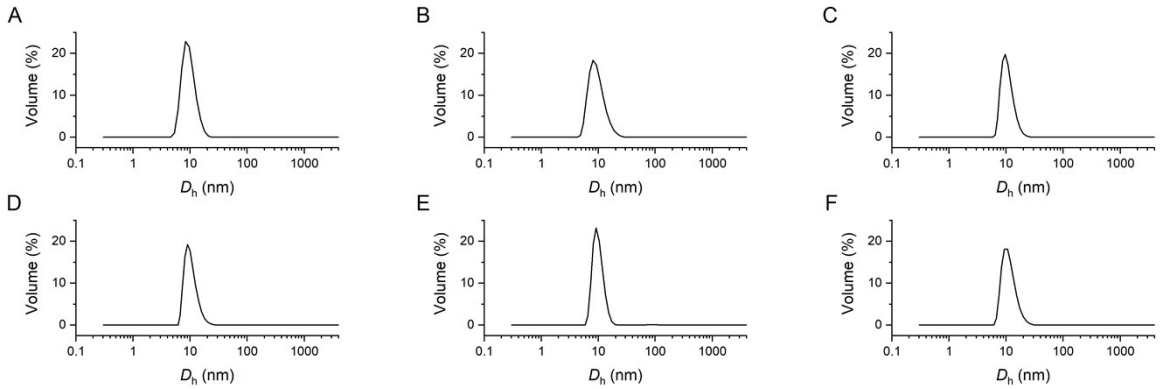

Figure S5 Hydrodynamic size distribution curves (D_h) of polymer samples corresponding to the data summarized in Table 1, measured by dynamic light scattering (DLS) in phosphate buffer (pH 7.4) at 25 °C. (A) **P1**, (B) **PNC**, (C) **PC**, (D) **P2**, (E) **PNC–Fe**, and (F) **PC–Fe.**

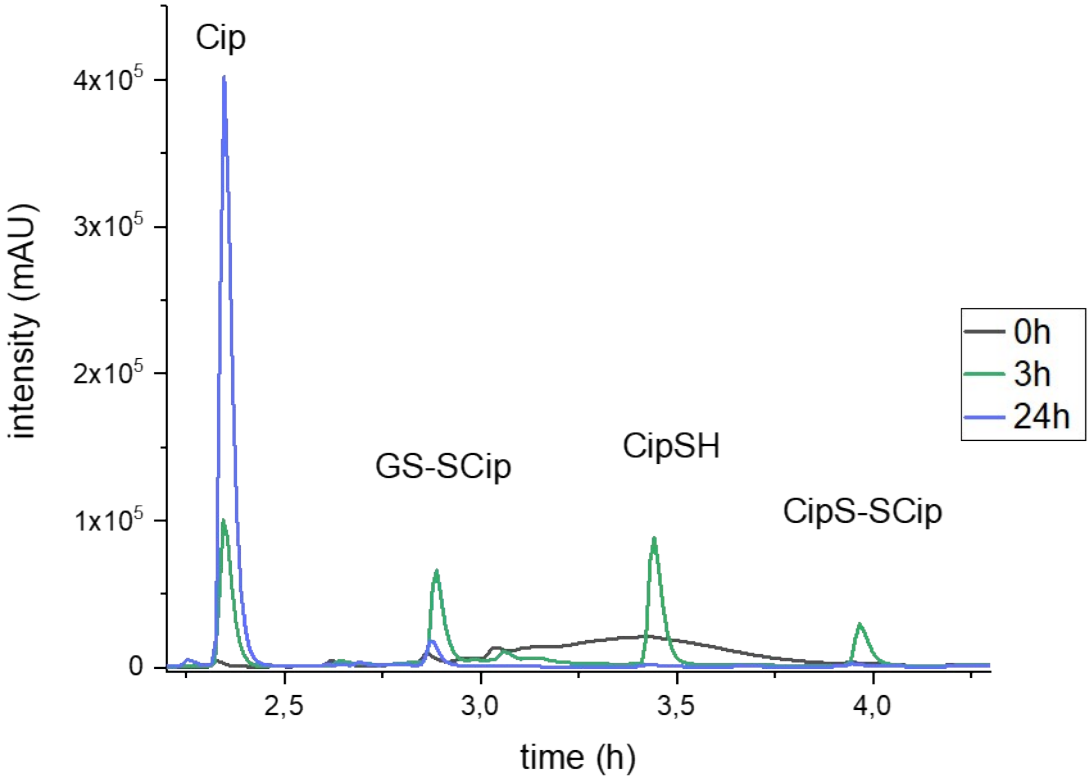

Figure S6 Overlay of HPLC chromatograms showing time-dependent release of ciprofloxacin from the **PC** conjugate upon GSH-mediated cleavage

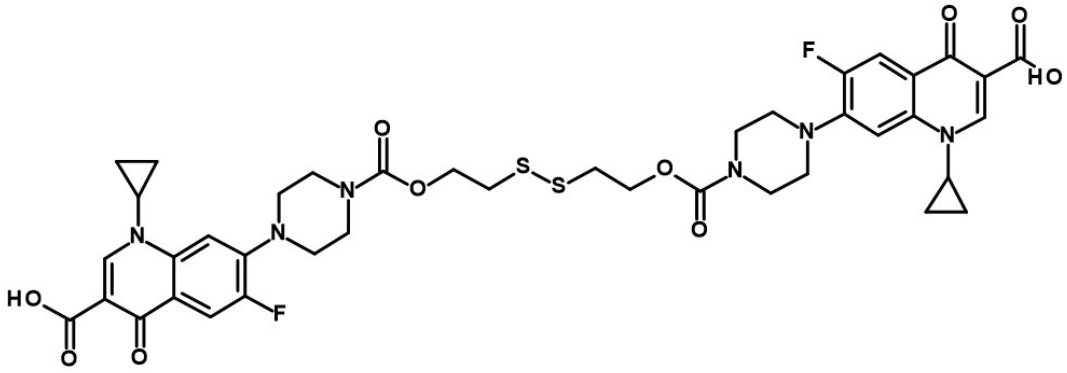

Figure S7 Structure of 7-[4-[2-[2-[4-(3-carboxy-1-cyclopropyl-6-fluoro-4-oxo-7-quinolyl)piperazine-1-carbonyl]oxyethyldisulfanyl]ethoxycarbonyl]piperazin-1-yl]-1-cyclopropyl-6-fluoro-4-oxo-quinoline-3-carboxylic acid (**CipSSCip**)

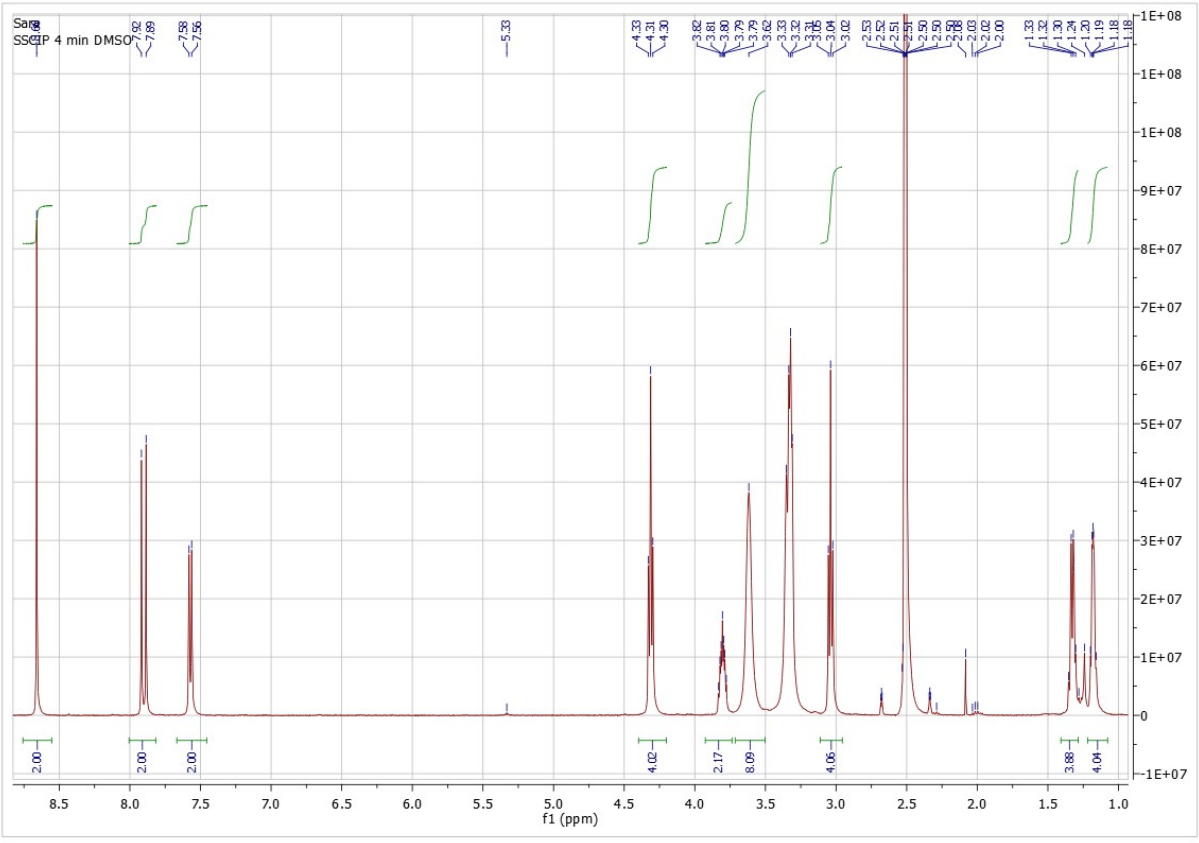

Figure S8 ^{1}H NMR spectrum of **CipSSCip** recorded in *d*6-DMSO at 400Mhz

Description of ^{1}H NMR spectra of the **CipSSCip**

^{1}H NMR (400 MHz, *d*6-DMSO): δ = 1.18 (m, 4H, CH_2-cyclopropyl; 1.32 (m, 4H, CH_2-cyclopropyl; 3.04 (t, 4H, CH_2S); 3.33 (m, 8H, CH_2N-piperazine); 3.62 (m, 8H, CH_2N-piperazine); 3.80 (septet, 2H, CH-cyclopropyl); 4.31 (t, 4H, CH_2O-linker); 7.57 (d, 2H, arom); 7.90 (d, 2H, arom-CHCF); 8.66 (s, 2H, arom-CHN); 15.15 (br, 2H, COOH) ppm.