

## Supporting information

# Potent Dual Inhibitors of Steroid Sulfatase and 17 $\beta$ -Hydroxysteroid Dehydrogenase Type 1 with a Suitable Pharmacokinetic Profile for in vivo Proof-of-Principle Studies in an Endometriosis Mouse Model

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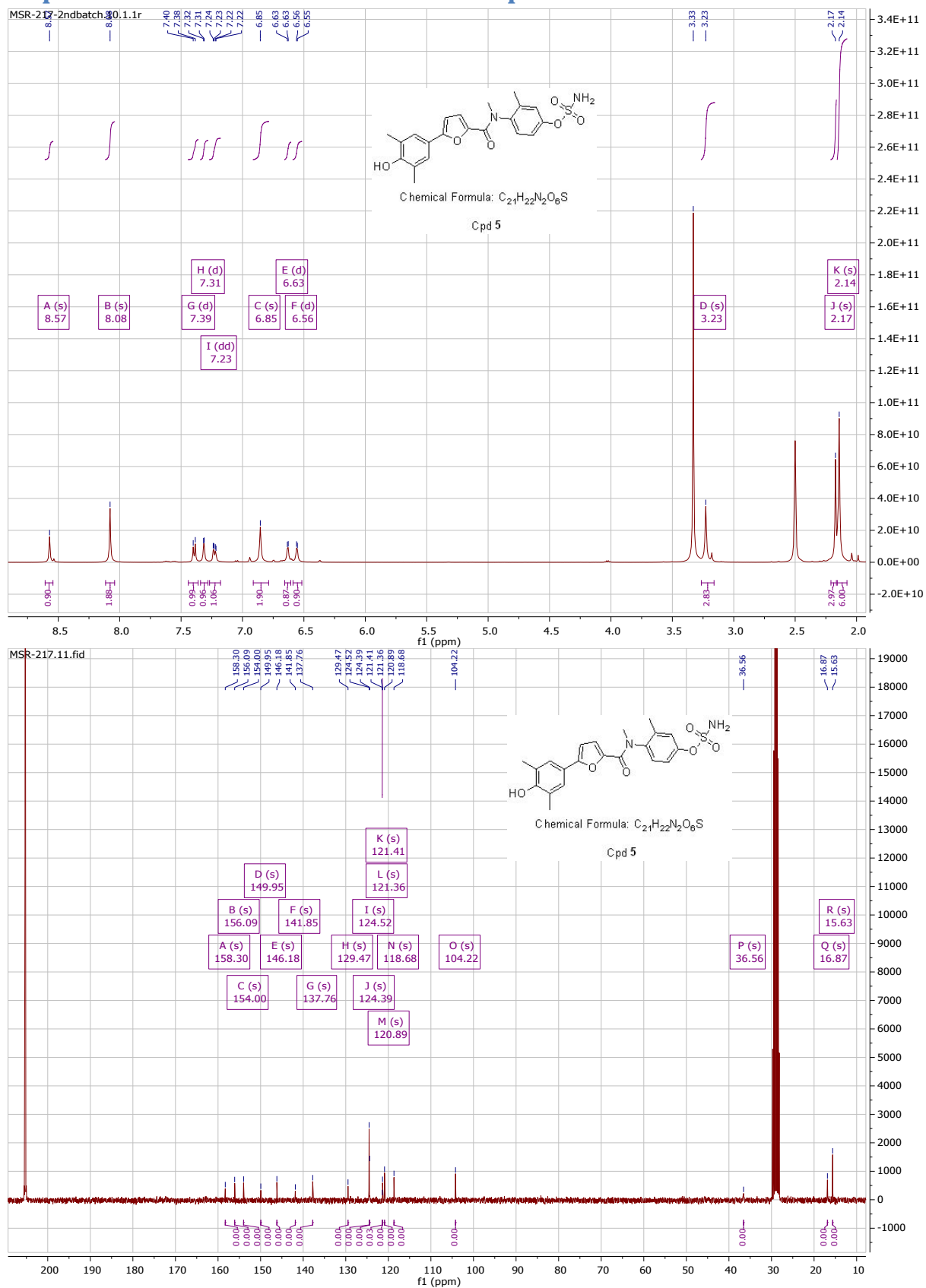
<sup>8</sup>Helmholtz Institute for Pharmaceutical Research Saarland (HIPS) - Helmholtz Centre for Infection Research (HZI), Department of Drug Design and Optimization, Campus Building E81, 66123 Saarbrücken, Germany

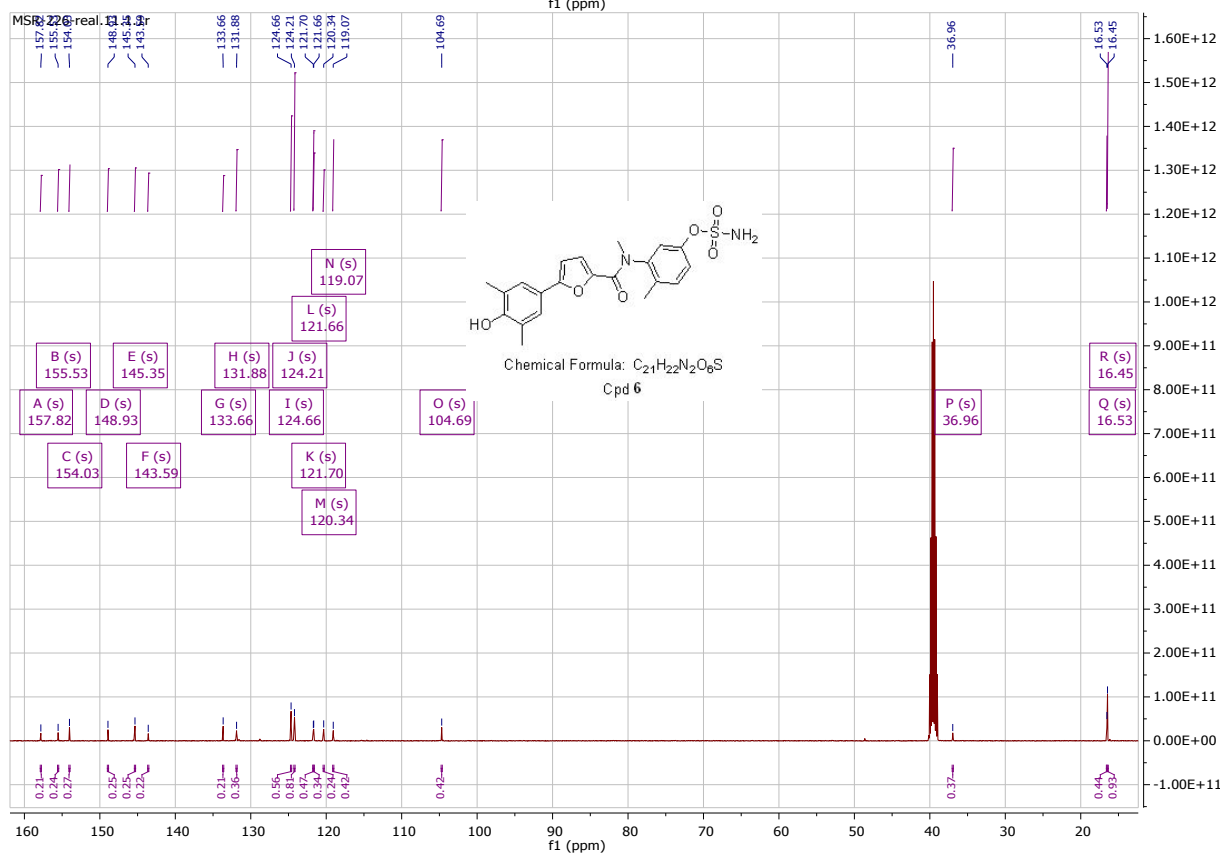
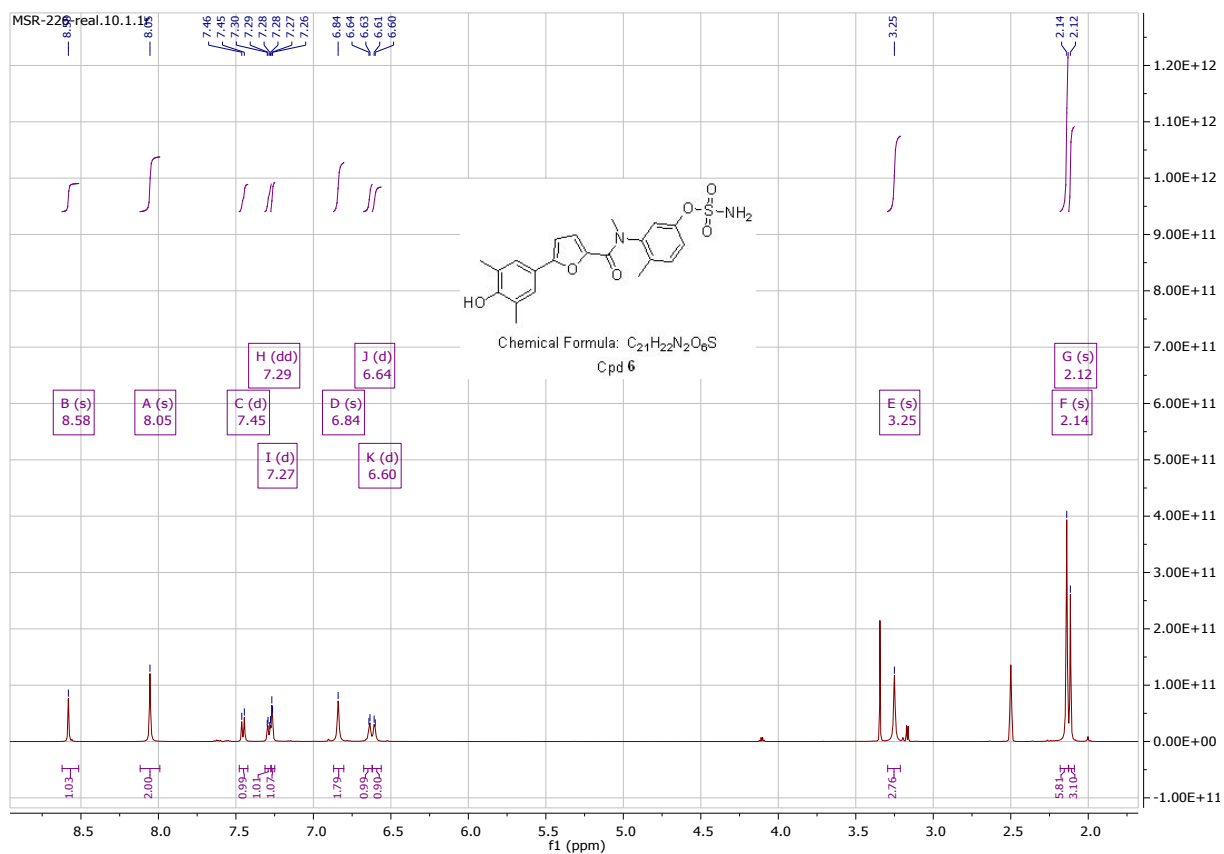
\*Martin Frotscher (email: m.frotscher@mx.uni-saarland.de)

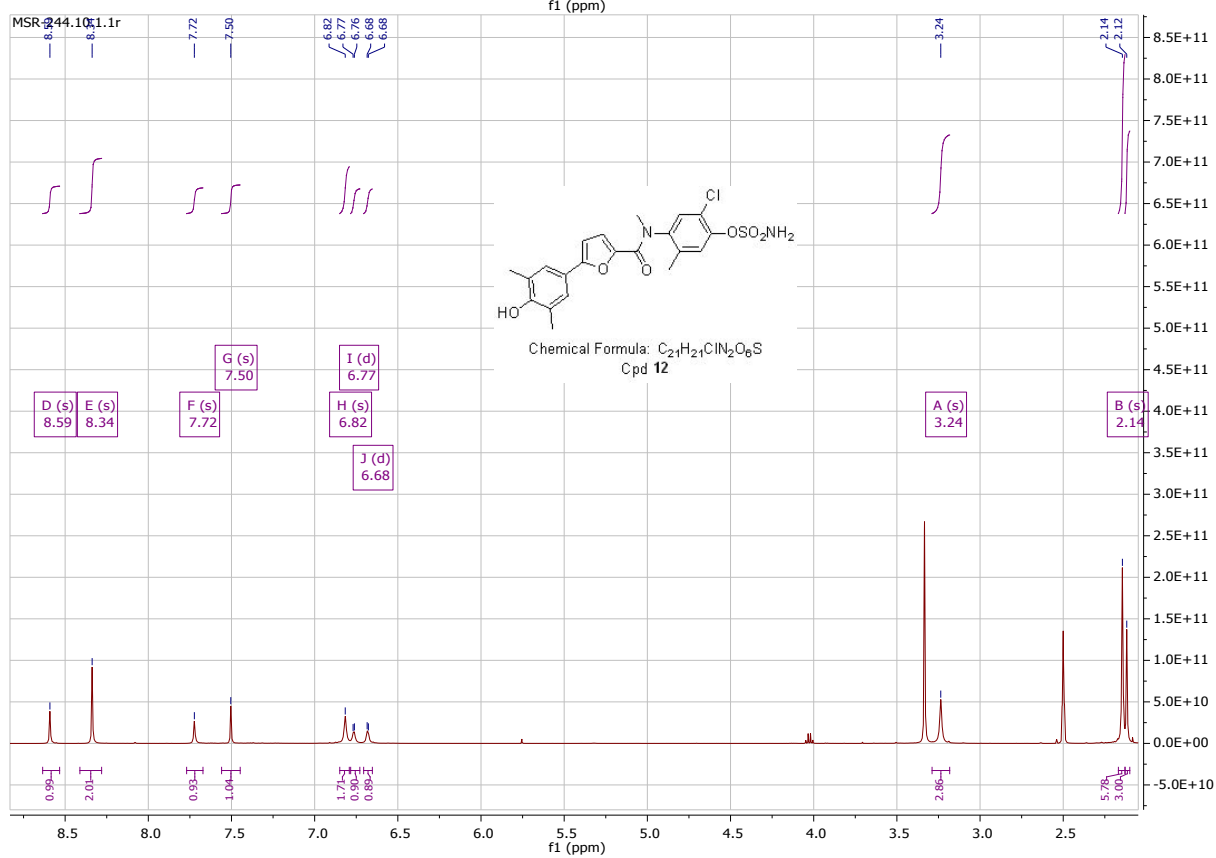
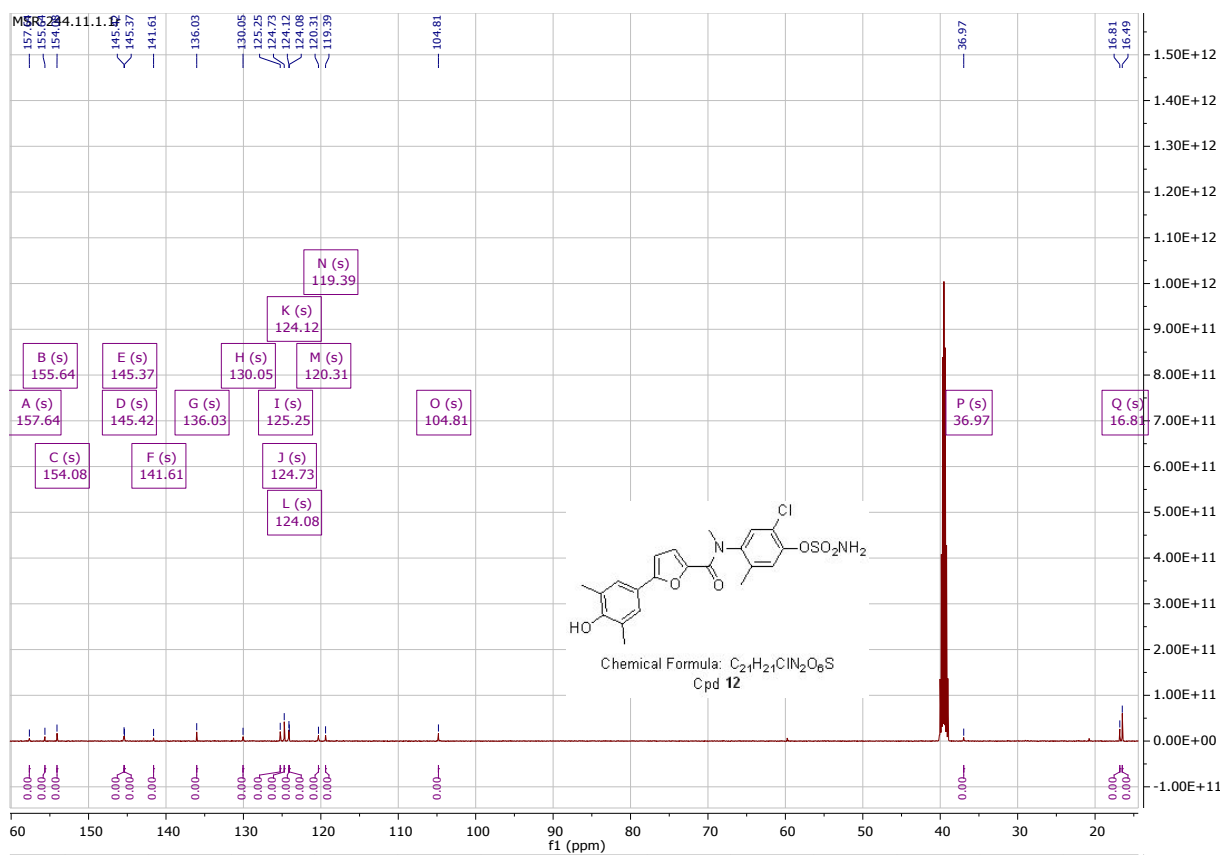
**Contents:**

Representative $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra.....	S3
Representative MS spectra and chromatograms.....	S6
Oral bioavailability of compound <b>5</b> .....	S8

## 1.1. Representative $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra





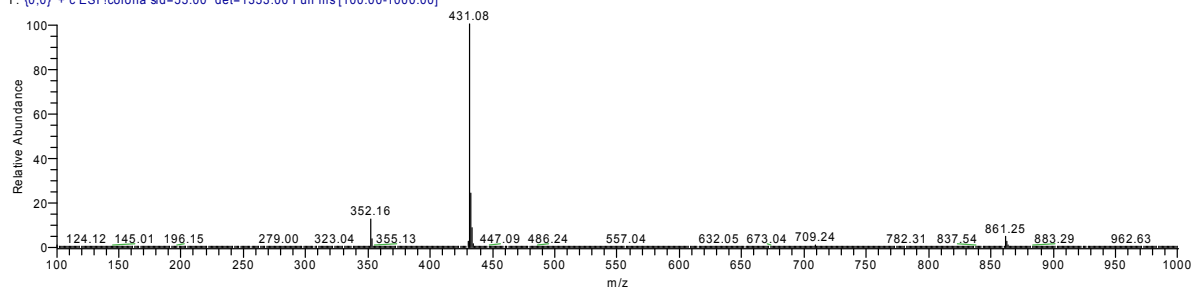


## 1.2.Representative MS spectra and chromatograms

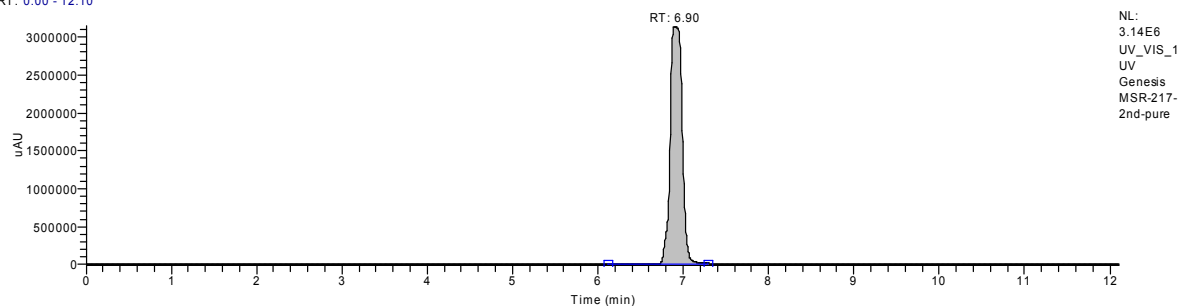
### Compound 5:

MSR-217-2nd-pure #345 RT: 7.32 AV: 1 NL: 2.38E7

T: [0.0] + c ESI Icorona sid=55.00 det=1353.00 Full ms [100.00-1000.00]



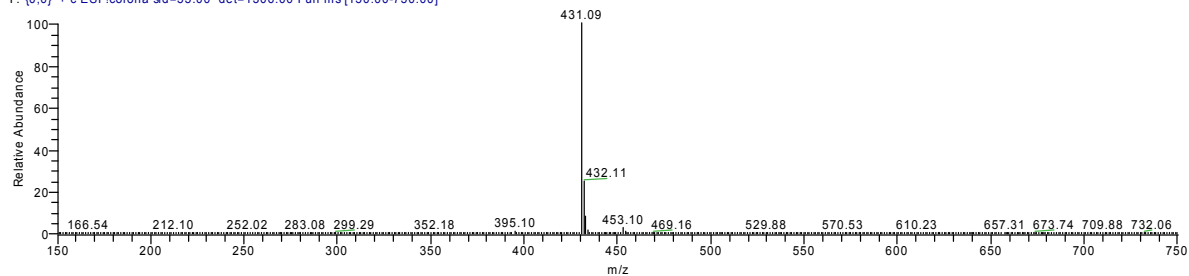
RT: 0.00 - 12.10



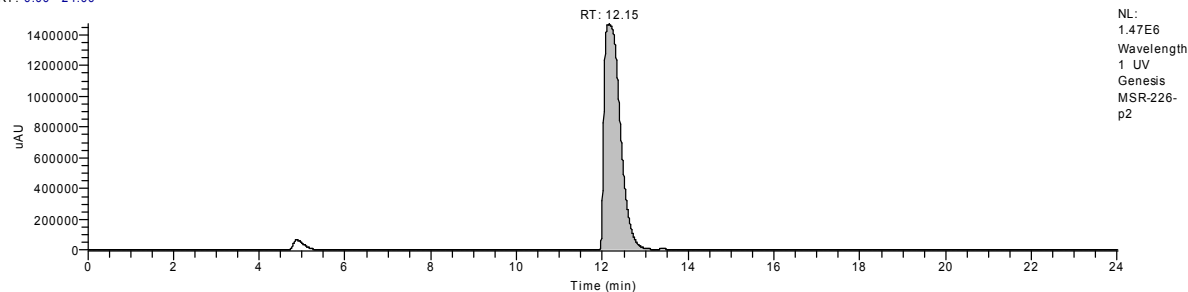
### Compound 6:

MSR-226-p2 #582 RT: 12.39 AV: 1 NL: 5.84E6

T: [0.0] + c ESI Icorona sid=55.00 det=1306.00 Full ms [150.00-750.00]

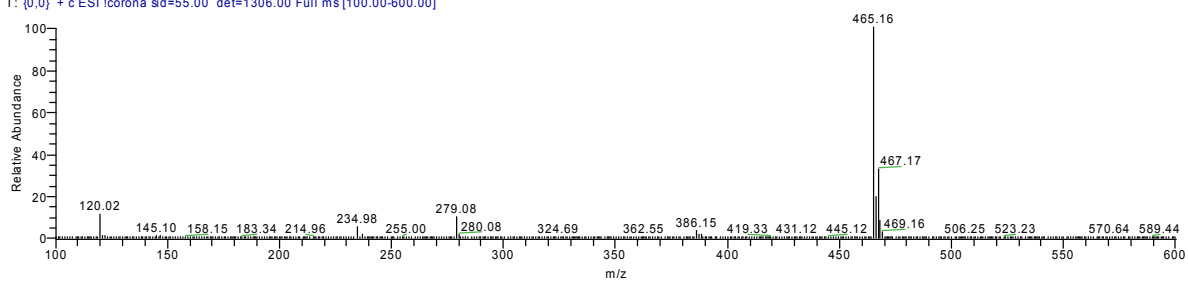


RT: 0.00 - 24.00

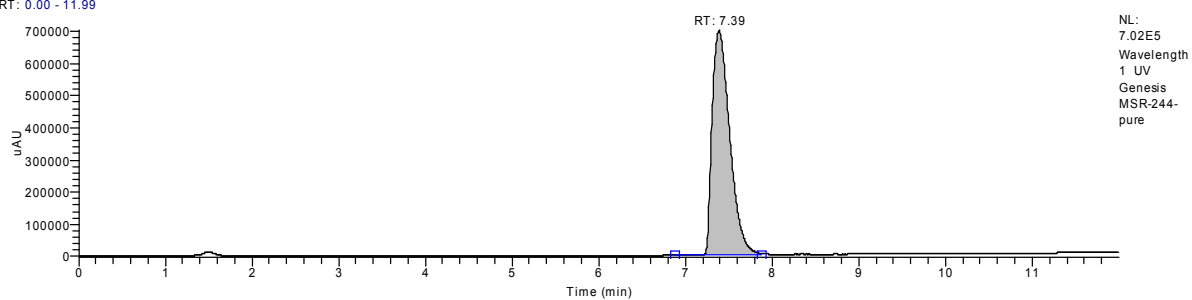


## Compound 12:

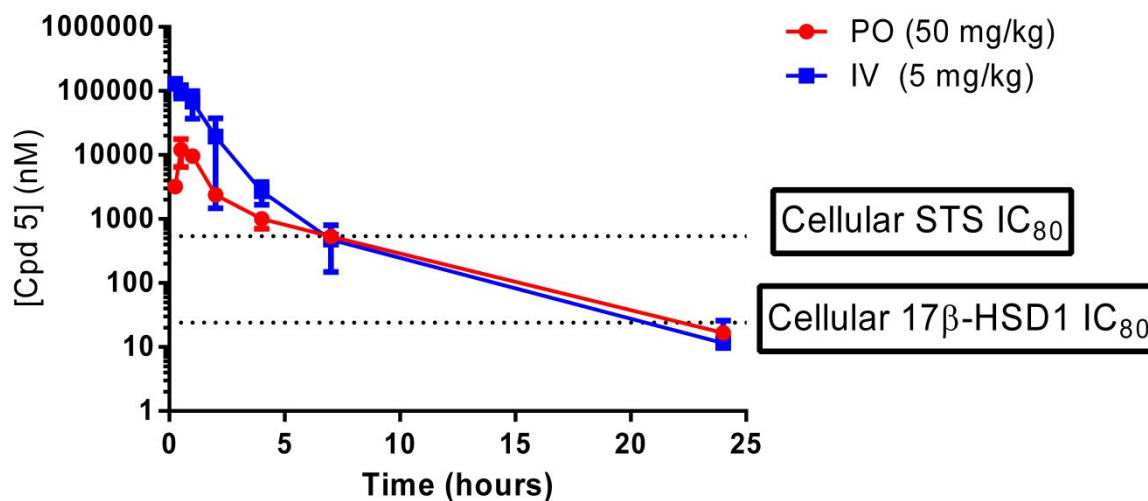
MSR-244-pure #464 RT: 7.56 AV: 1 NL: 2.41E6  
T: [0.0] + c ESI Icorona sid=55.00 det=1306.00 Full ms [100.00-600.00]



RT: 0.00 - 11.99



## 2. Oral bioavailability of compound **5**



**Figure S1.** Mean profile ( $\pm$ SD) of plasma concentration [nM] in C57BL/6 mice vs time after oral (50 mg/kg) and intravenous (5 mg/kg) application of compounds **5** in single dosing experiments (n=3). Dotted lines represent the cellular  $IC_{80}$  values of compound **5** for STS and 17 $\beta$ -HSD1 values .

Oral bioavailability (%F) of compound **5**

$$\%F = \frac{AUC_{po} * Dose_{iv}}{AUC_{iv} * Dose_{po}} * 100 = \frac{10350 * 5}{69933 * 50} * 100 = 1.47\%$$