

Supplementary Information

Highly enantioselective bioreduction of 1-(3,4-difluorophenyl)-3-nitropropan-1-one: Key intermediate of Ticagrelor

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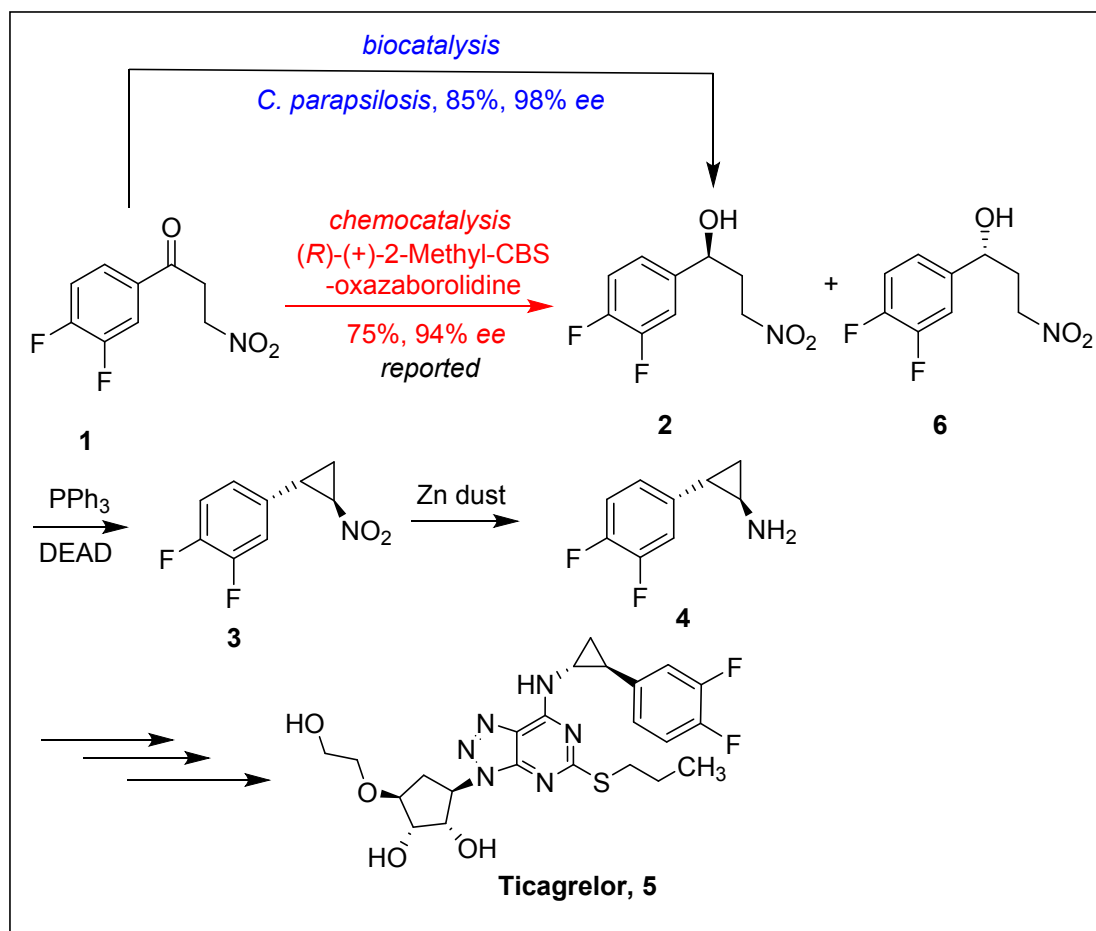
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Scheme 1



1. HPLC Methods

a) Purity by HPLC: Standard

Determined by HPLC using Zorbex Eclipse Plus C-18 at 210 nm. Mobile phase consisted of A: 0.02 M KH_2PO_4 buffer pH 3.0 and B: ACN:H₂O (90:10 v/v).

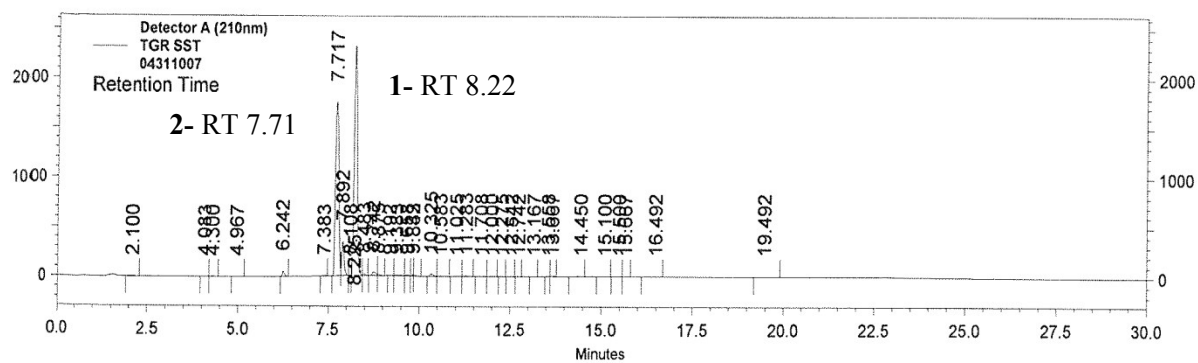


Figure S1: HPLC spectrum of standard substrate (1) and product (2).

b) Purity by HPLC: 1-(3,4-difluorophenyl)-3-nitropropan-1-ol

Determined by HPLC using Zorbex Eclipse Plus C-18 at 210 nm. Mobile phase consisted of A: 0.02 M KH_2PO_4 buffer pH 3.0 and B: ACN:H₂O (90:10 v/v).

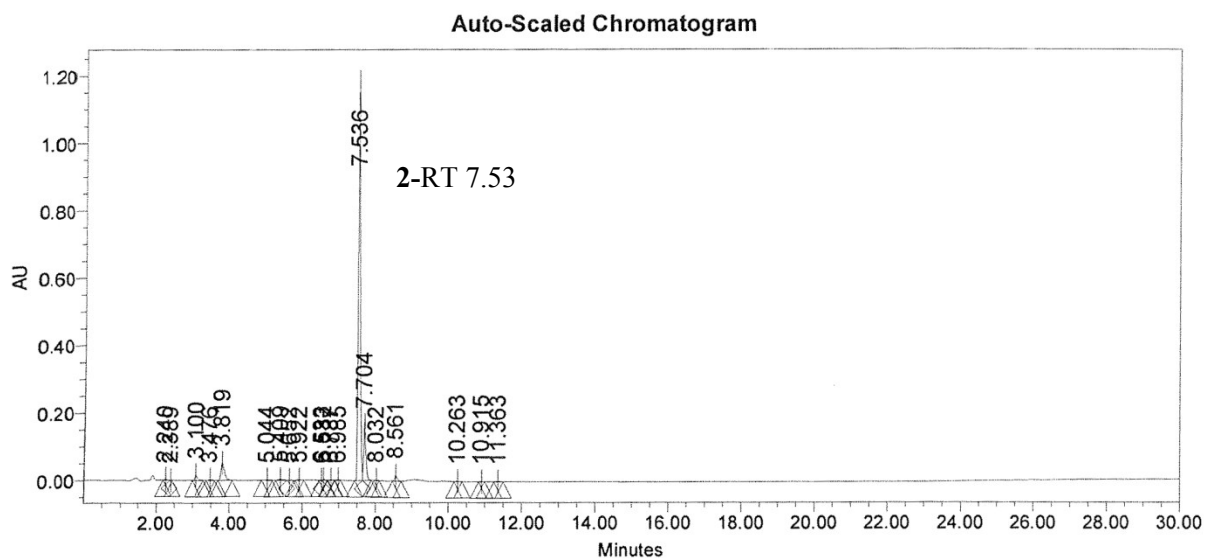


Figure S2: HPLC spectrum of preparative scale batch 1-(3,4-difluorophenyl)-3-nitropropan-1-ol (**2**).

c) Chiral HPLC: Standards (1) (2) and (6)

Determined by using chiral HPLC column Chiralcel OD-H at 210 nm. Mobile phase consisted of Hexane/*i*PrOH/TFA (92:7.9:0.1).

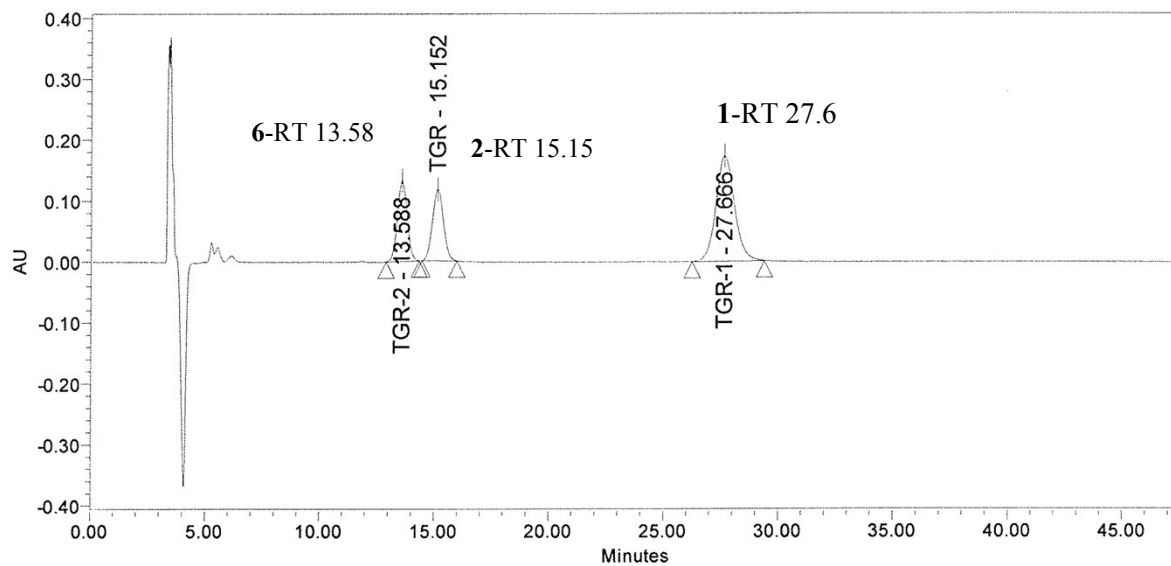


Figure S3: Chiral HPLC spectrum of standard (1) (2) and (6).

d) Chiral HPLC: Preparative batch sample

Determined by using chiral HPLC column Chiralcel OD-H at 210 nm. Mobile phase consisted of Hexane/iPrOH/TFA (92:7.9:0.1).

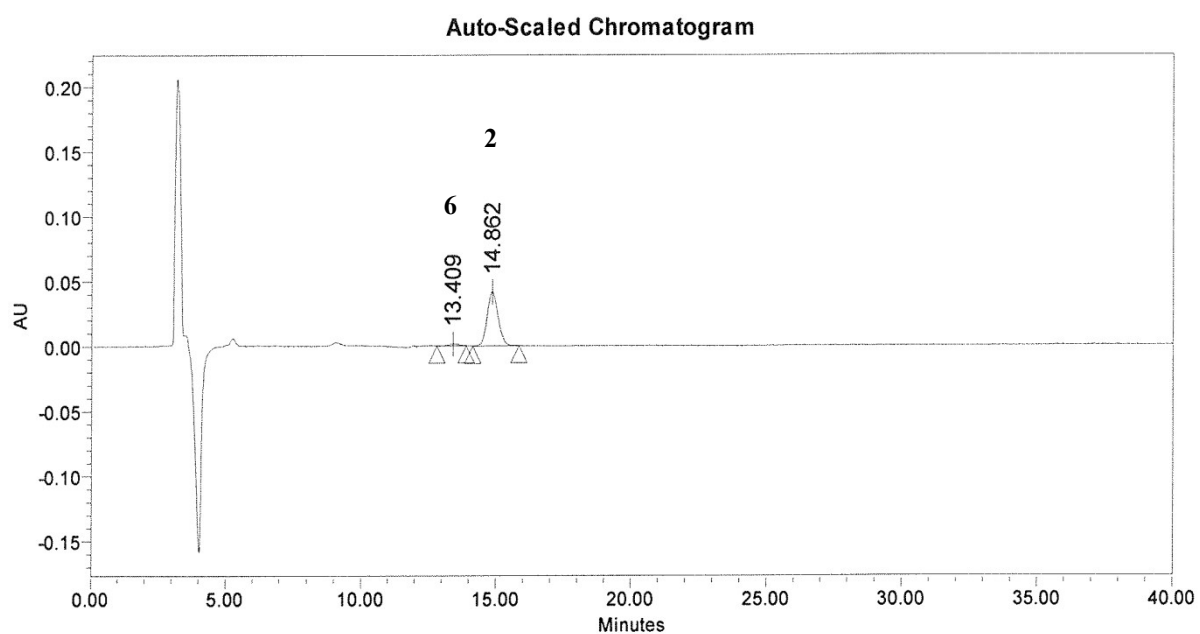


Figure S4: Chiral HPLC spectrum of preparative batch showing (1), (2) and (6)

2. NMR spectra

a) ¹H-NMR spectra: 1-(3,4-Difluorophenyl)-3-nitropropan-1-one

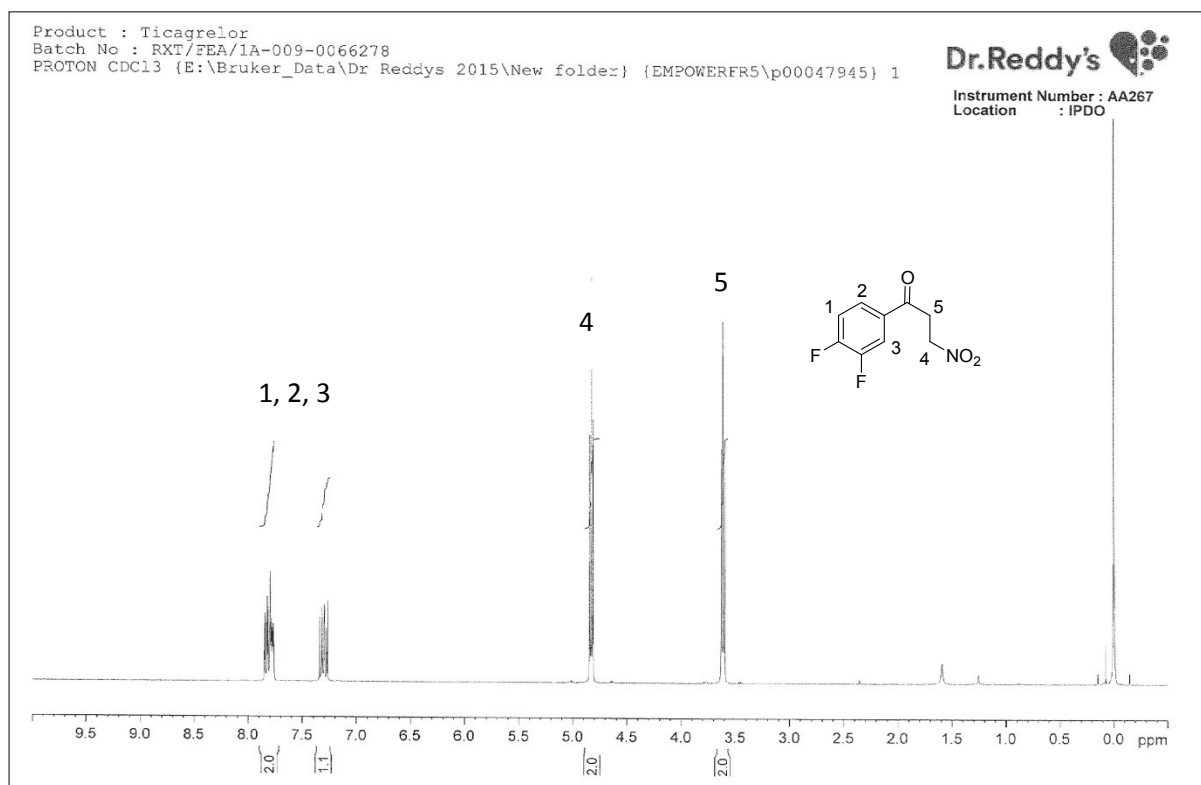


Figure S5: ¹H NMR spectrum of 1-(3,4-difluorophenyl)-3-nitropropan-1-one in CDCl₃.

b) $^{13}\text{H-NMR}$ spectra: 1-(3,4-Difluorophenyl)-3-nitropropan-1-one

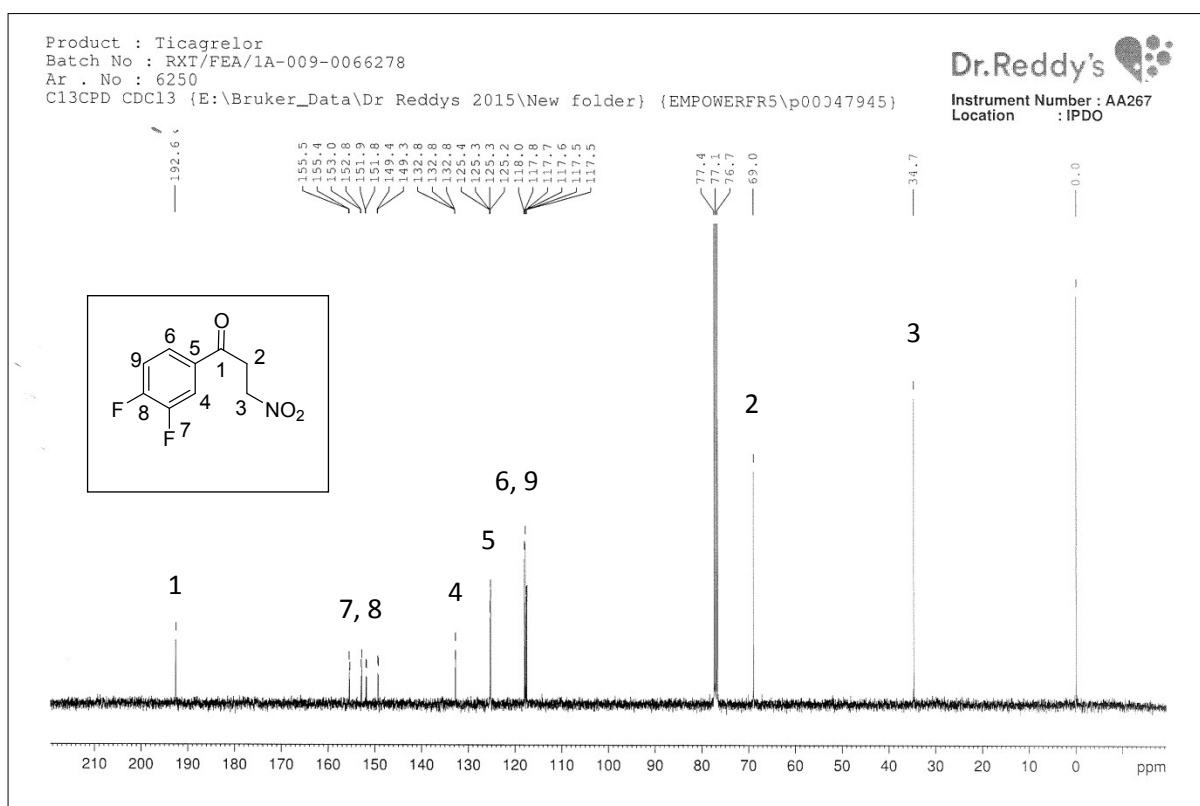


Figure S6: ^{13}C NMR spectrum of (S)-1-(3,4-difluorophenyl)-3-nitropropan-1-ol in CDCl_3 .

c) ^1H -NMR spectra: 1-(3,4-difluorophenyl)-3-nitropropan-1-ol

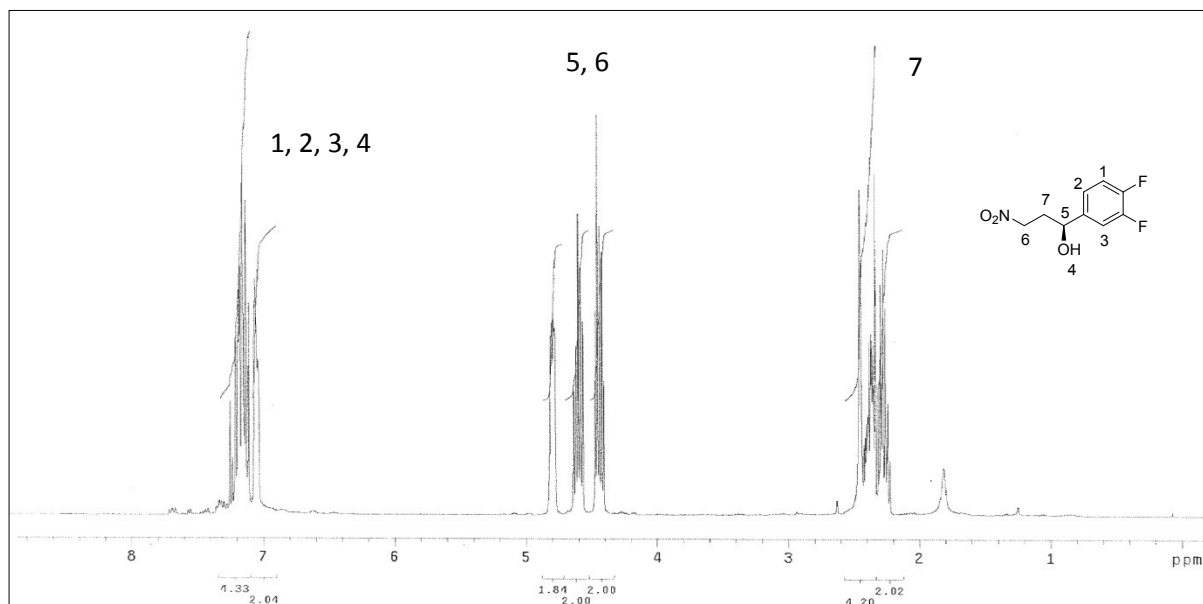


Figure S7: ^1H NMR spectrum of (S)-1-(3,4-difluorophenyl)-3-nitropropan-1-ol in CDCl_3 .

3. Mass Spectrum: 1-(3,4-difluorophenyl)-3-nitropropan-1-ol

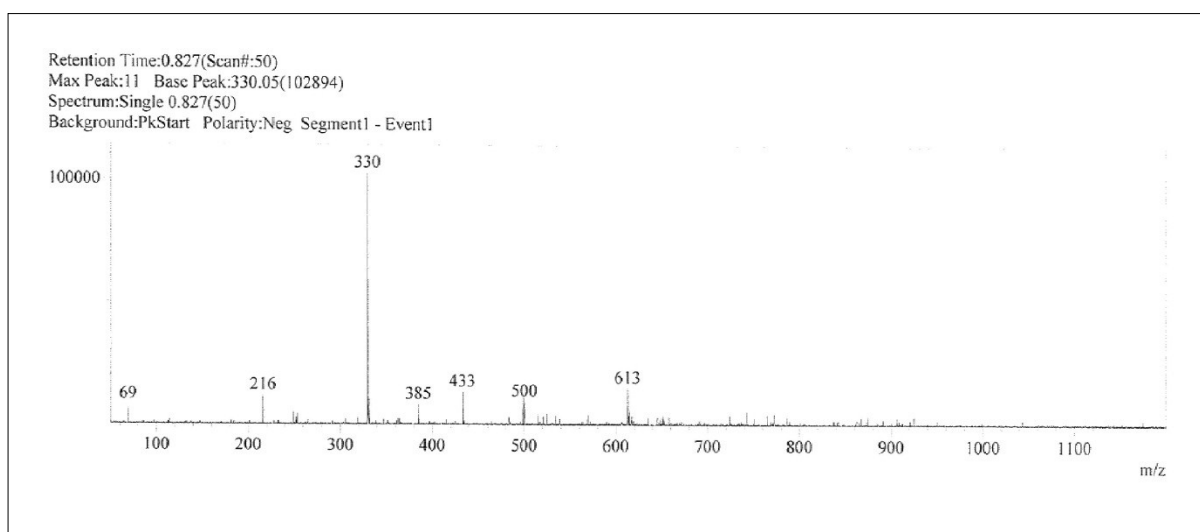


Figure S8: Mass (M-H) spectrum of (*S*)-1-(3,4-difluorophenyl)-3-nitropropan-1-ol.

4. IR Spectrum: (S)-1-(3,4-difluorophenyl)-3-nitropropan-1-ol

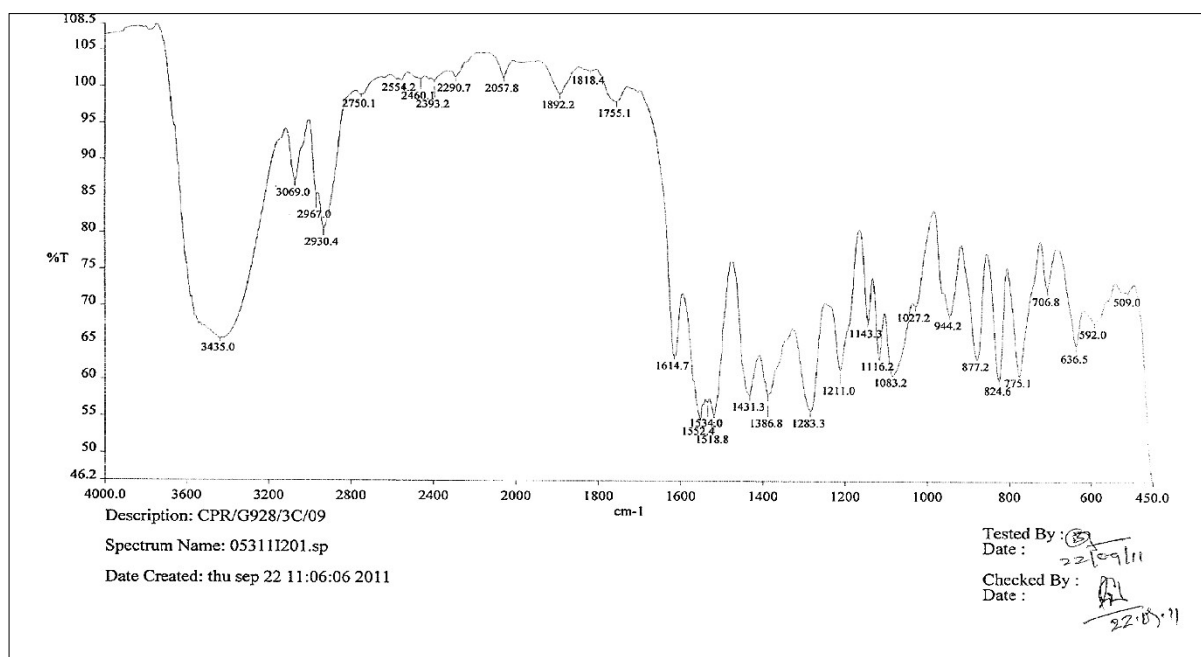


Figure S9: IR spectrum of (S)-1-(3,4-difluorophenyl)-3-nitropropan-1-ol.