

Supporting information for

Stereocontrolled Synthesis and Investigation of the biosynthetic transformations of 16(S),17(S)-epoxy-PD_{n-3}DPA

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General Information

Unless stated otherwise, all commercially available reagents and solvents were used in the form they were supplied without any further purification. The stated yields are based on isolated material. All reactions were performed under an argon atmosphere using Schlenk techniques. Reaction flasks were covered with aluminium foil during reactions and storage to minimize exposure to sunlight. Thin layer chromatography was performed on silica gel 60 F₂₅₄ aluminum-backed plates fabricated by Merck. Flash column chromatography was performed on silica gel 60 (40-63 µm) produced by Merck. NMR spectra were recorded on a Bruker AVI600, Bruker AVII400 or a Bruker DPX300 spectrometer at 600 MHz, 400 MHz or 300 MHz respectively for ¹H NMR and at 150 MHz, 100 MHz or 75 MHz respectively for ¹³C NMR. Coupling constants (*J*) are reported in hertz and chemical shifts are reported in parts per million (δ) relative to the central residual protium solvent resonance in ¹H NMR (CDCl₃ = δ 7.26, DMSO-*d*₆ = δ 2.50, benzene-*d*₆ = δ 7.16 and MeOD-*d*₄ = δ 3.31 ppm) and the central carbon solvent resonance in ¹³C NMR (CDCl₃ = δ 77.00, DMSO-*d*₆ = δ 39.43, benzene-*d*₆ = δ 128.06 and MeOD-*d*₄ = δ 49.00 ppm). Mass spectra were recorded at 70 eV on Micromass Prospec Q or Micromas QTOF 2W spectrometer using EI, ES or CI as the methods of ionization. High resolution mass spectra were recorded on Micromass Prospec Q or Micromas QTOF 2W spectrometer using EI or ES as the methods of ionization. Optical rotations were measured using a 0.7 mL cell with a 1.0 dm path length on an Anton Paar MCP 100 polarimeter. HPLC analyses were performed on an Agilent Technologies 1200 Series instrument with diode array detector set at 254 nm and equipped with a C18 stationary phase (Eclipse XDB-C18 5 µm 4.6 × 150 mm), applying the conditions stated. GLC analyses were performed on an Agilent 7820A with a FID detector, HP-5 capillary column, with helium as the carrier gas and by applying the conditions stated.

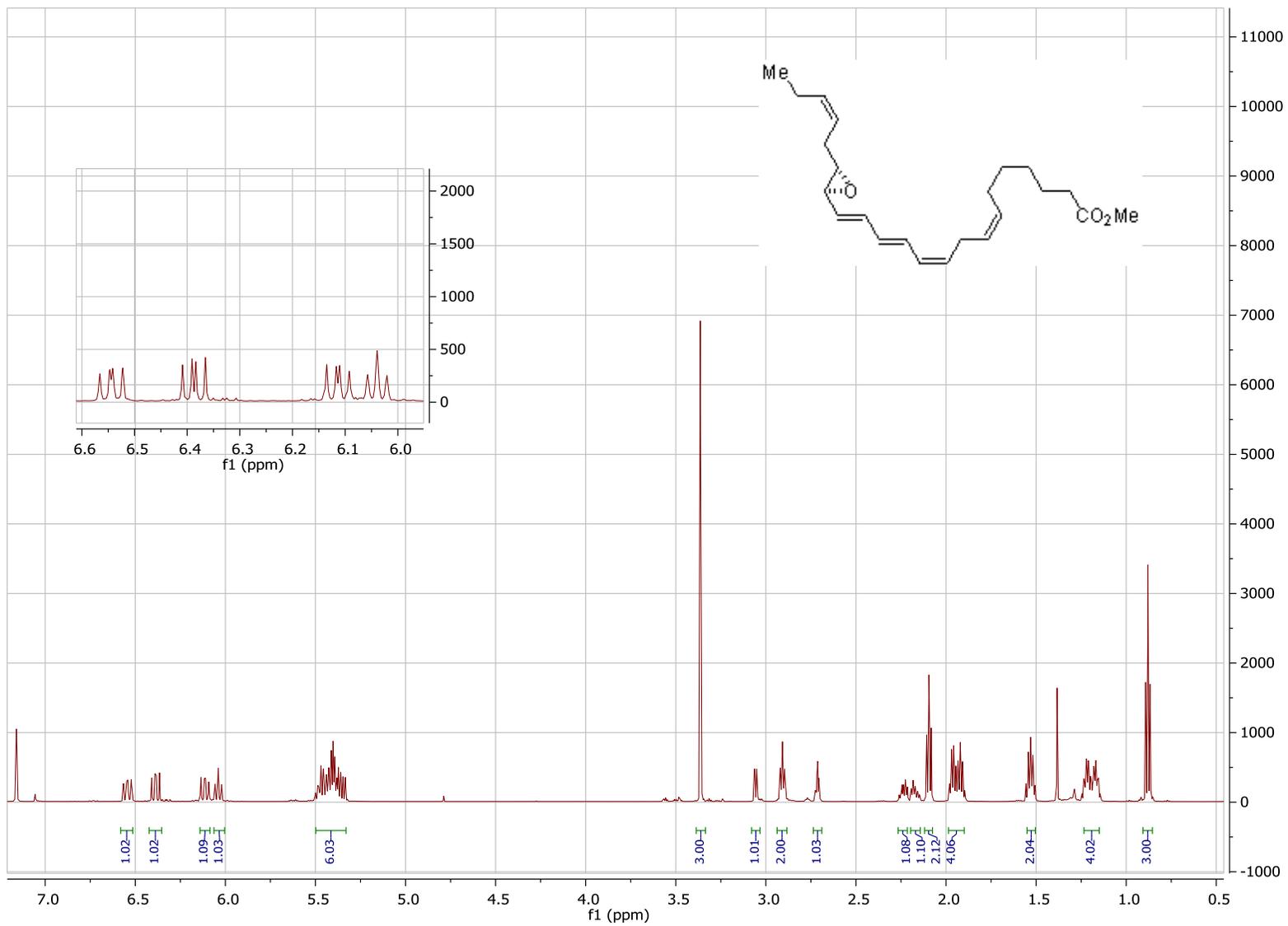


Figure S-1 $^1\text{H-NMR}$ spectrum of methyl ester (13).

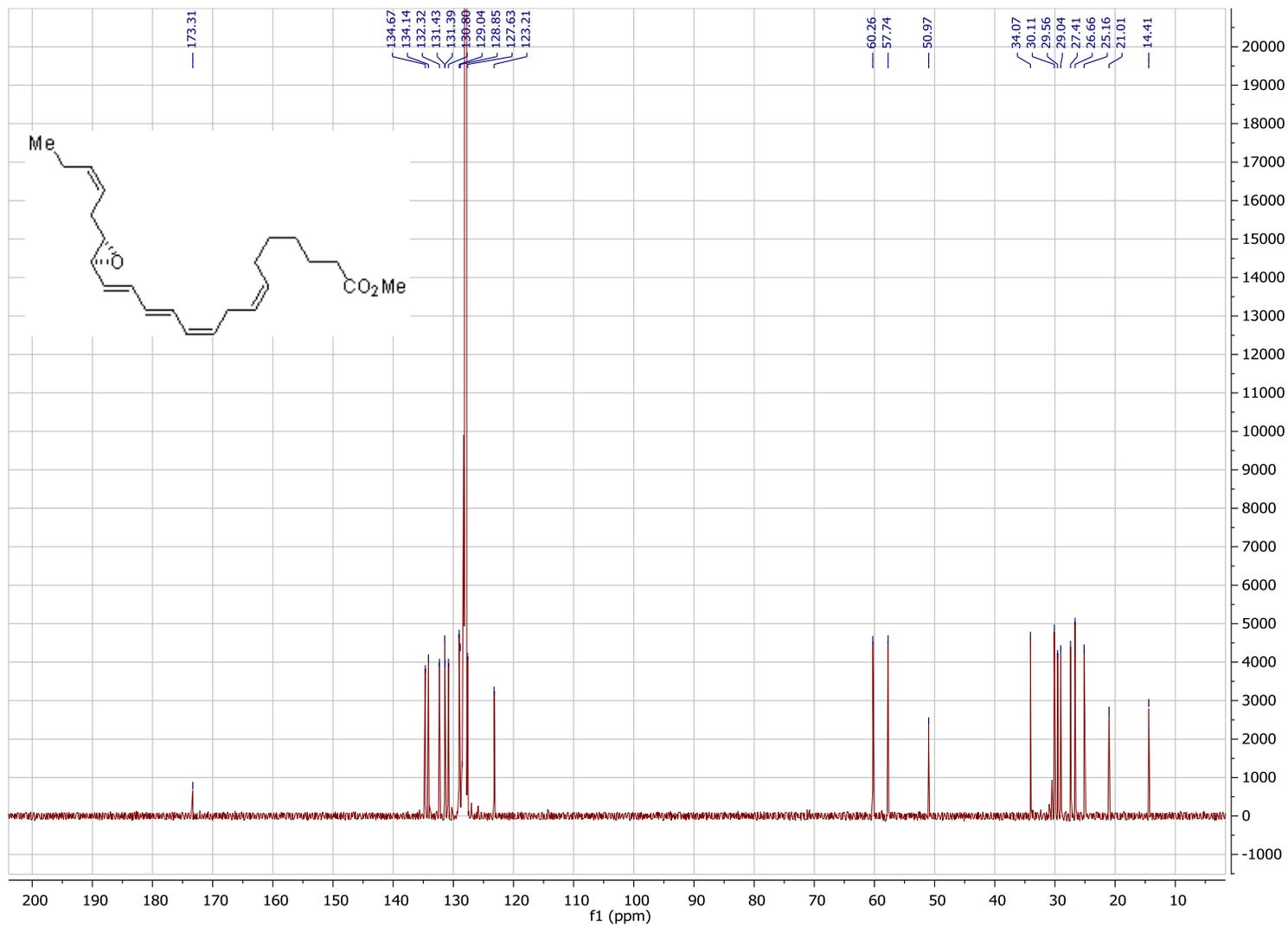


Figure S-2 ^{13}C -NMR spectrum of methyl ester (13).

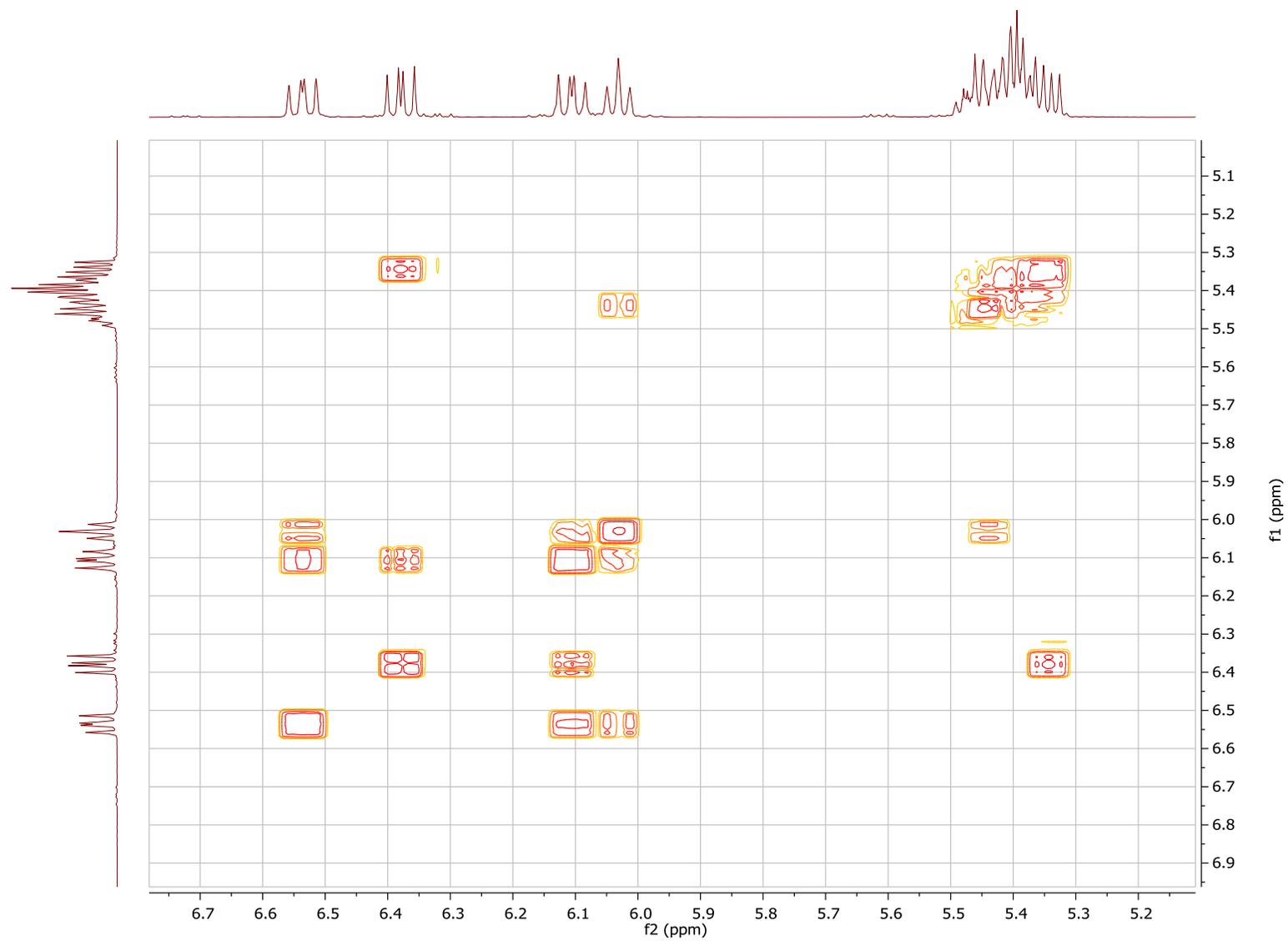


Figure S-3 COSY spectrum of methyl ester (**13**).

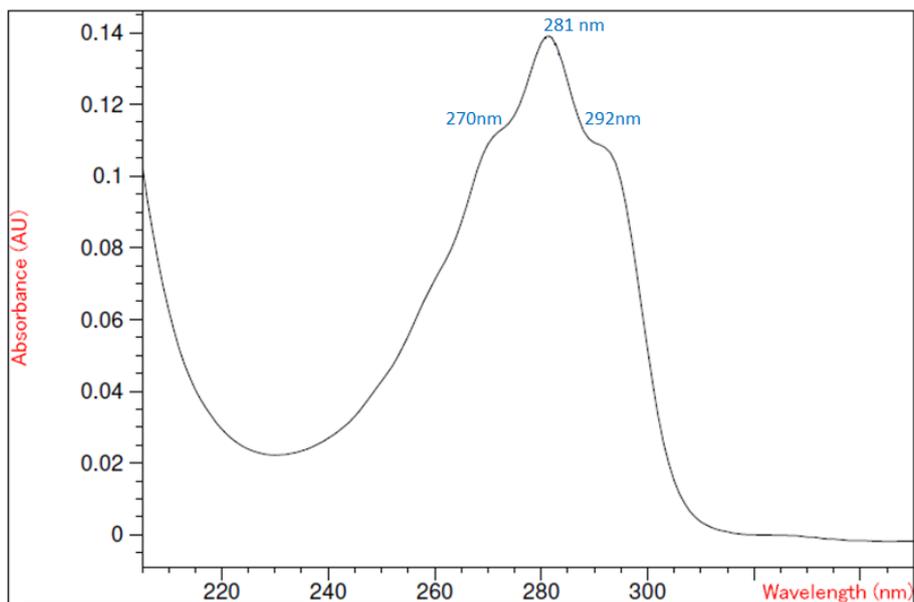


Figure S-4 UV-Vis chromatogram of the methyl ester **13**.

Elemental Analysis Report

Analysis Info	Acquisition Date	10/20/2016 10:56:29 AM
Sample Name	Analysis Name	D:\Data\maxis2016\12053.d
Method	ESI_pos_50_1500.m	

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

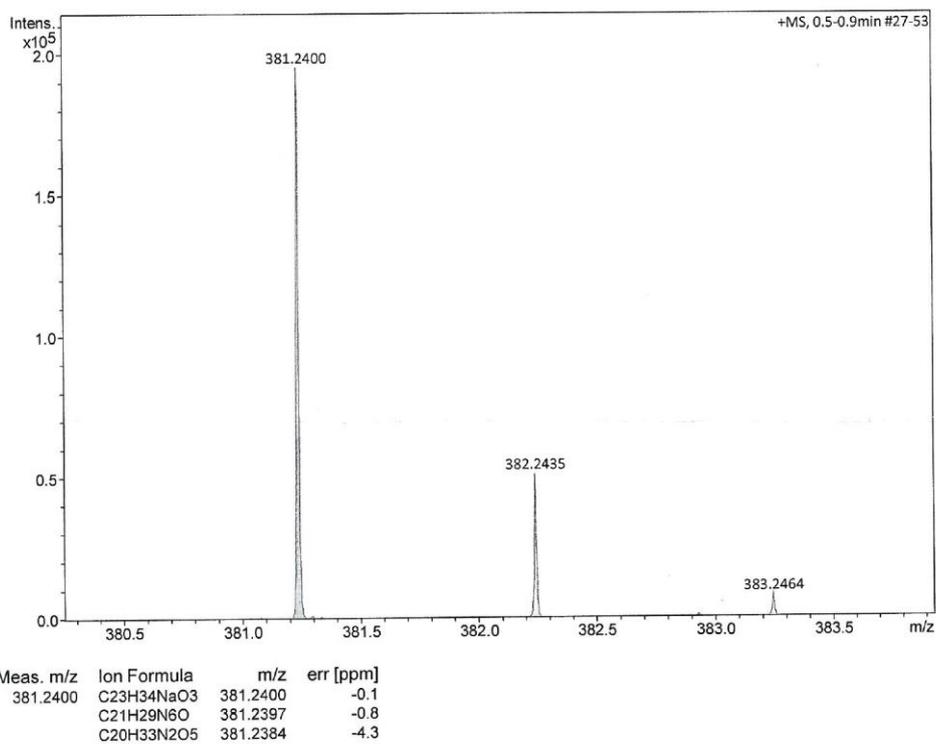


Figure S-5 HRMS of the methyl ester **13**.