Supporting information

Total Synthesis of the Antidiabetic (type 2) Lipid Mediator Protectin DX/PDX

Jean-Yves Sancéau*[†], René Maltais[†], Donald Poirier[†‡] and André Marette [±]

[†]*Organic Synthesis Service, Medicinal Chemistry Platform, Centre Hospitalier Universitaire (CHU) de Québec-Research Center, Québec, QC, Canada*

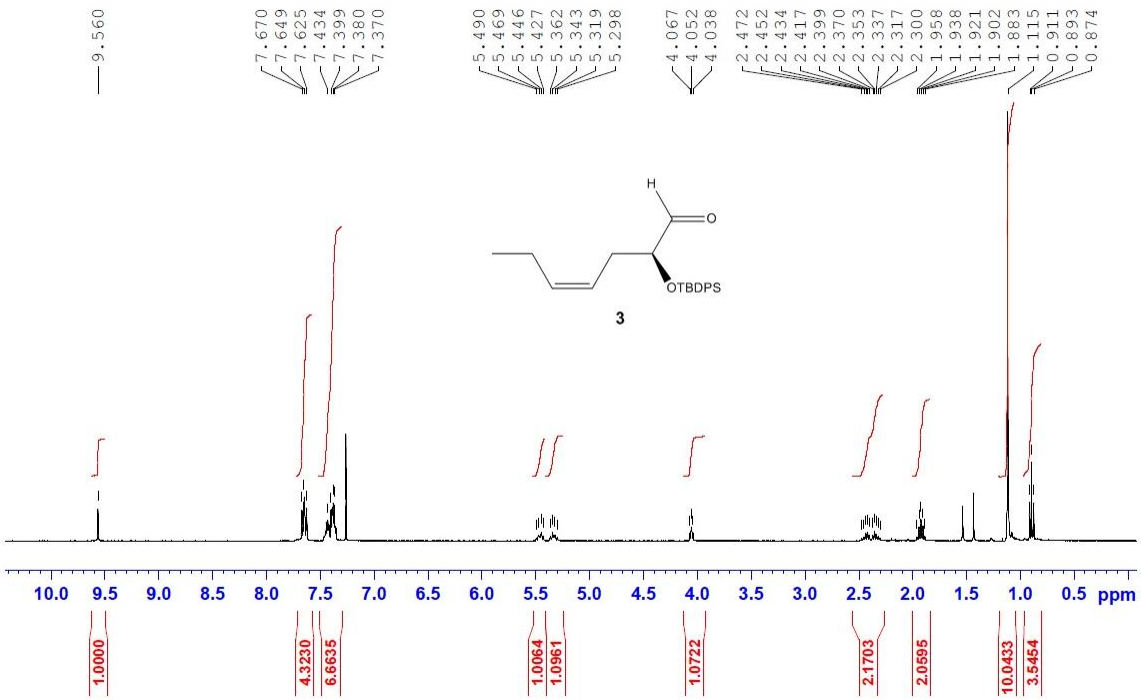
[‡]*Department of Molecular Medicine, Faculty of Medicine, Université Laval, Québec, QC, Canada*

[±] *Department of Medicine, Québec Heart and Lung Institute, Laval Hospital, Québec, QC, Canada*

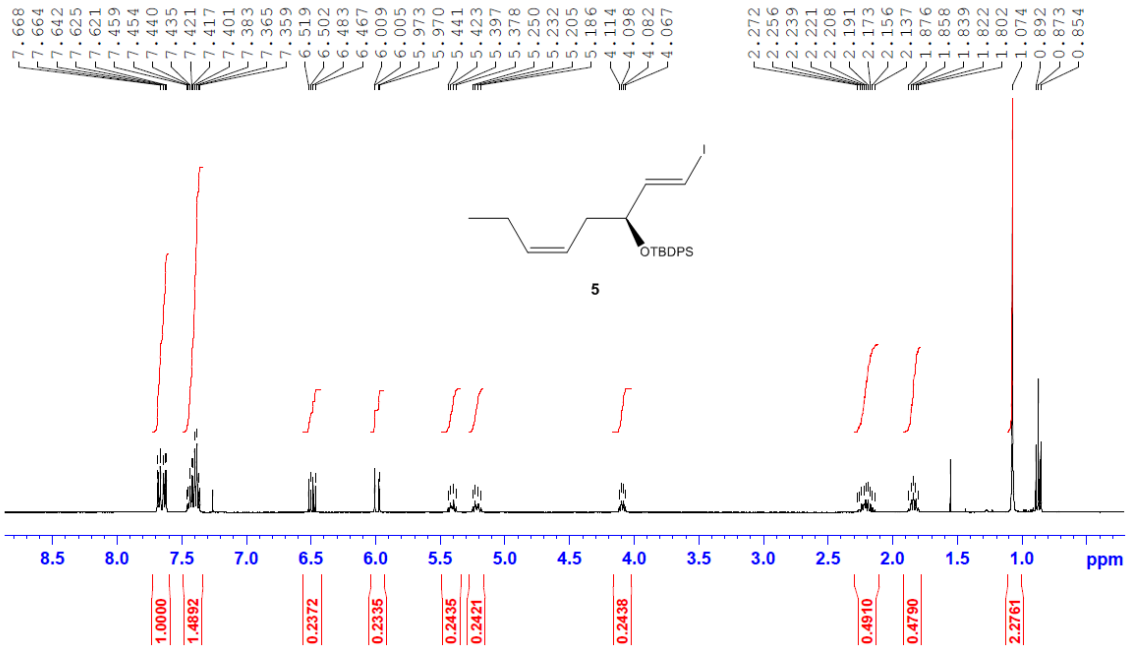
Contents

1. NMR spectra of **3**, **5-8**, **12**, **13**, **15-23**, PDX-methyl ester (**24**) and PDX (**2**)

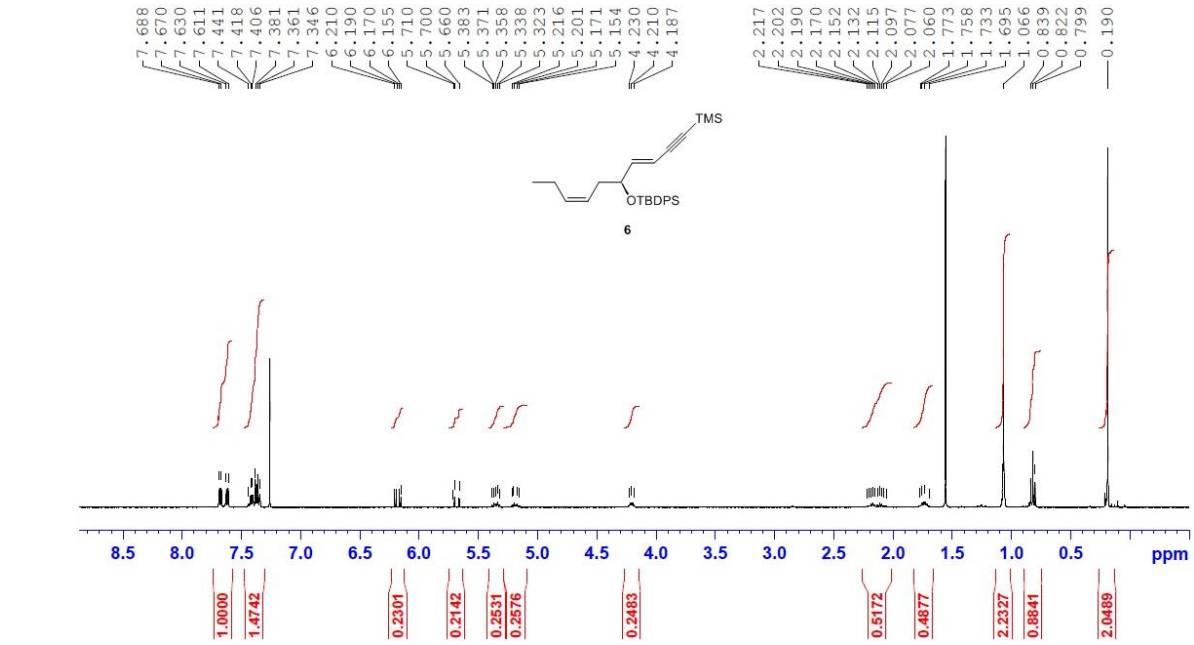
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**

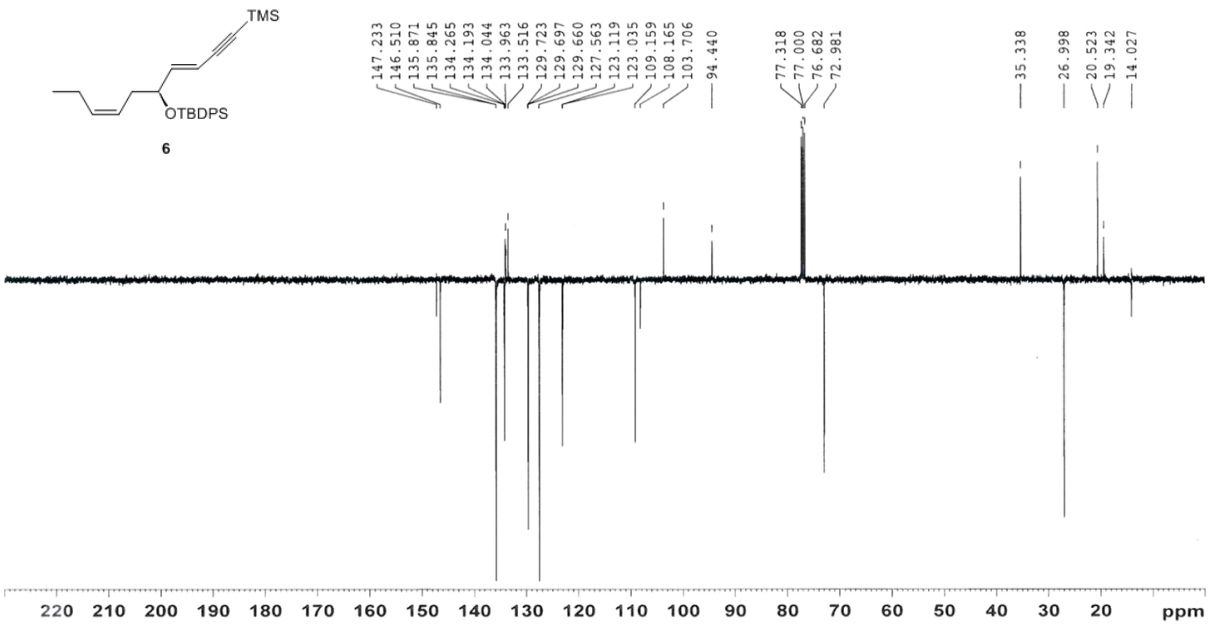


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**

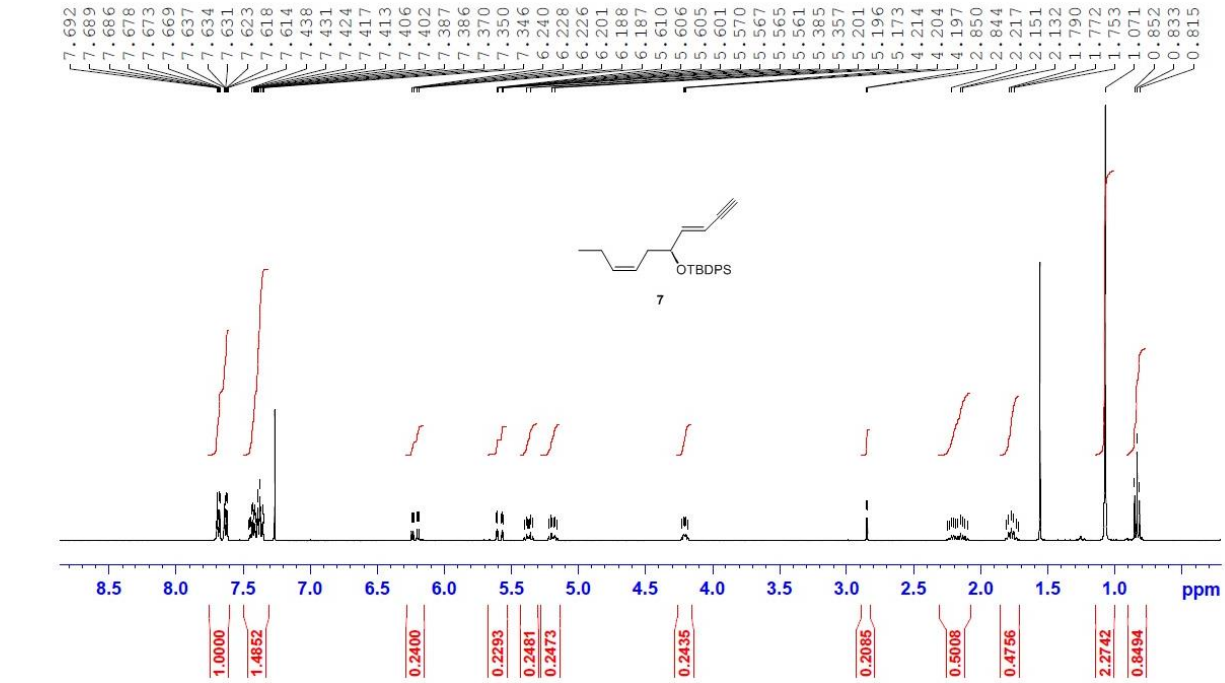


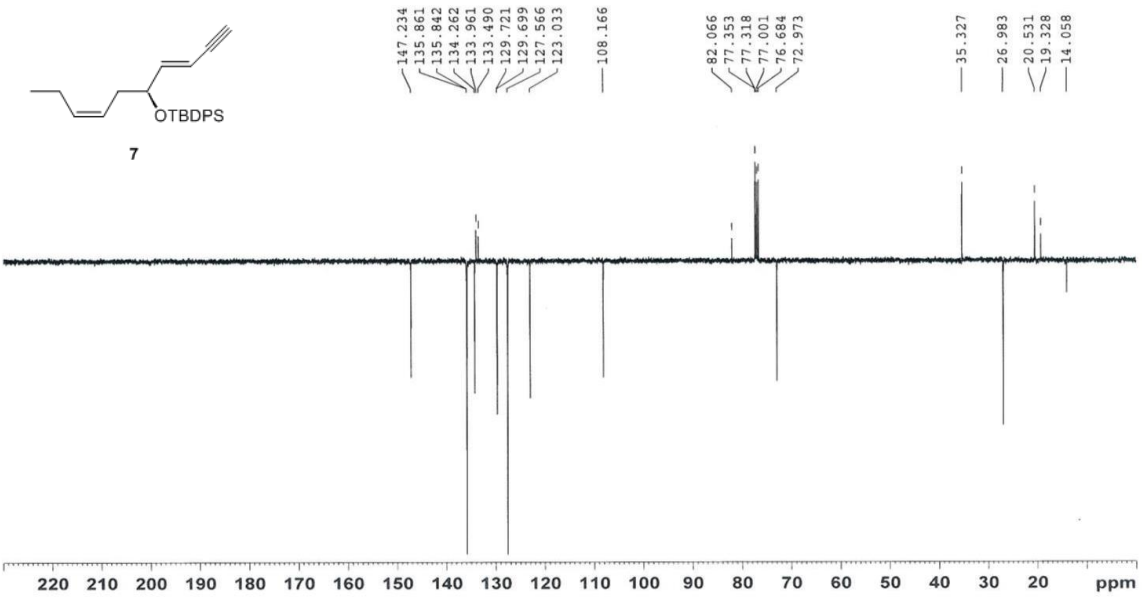
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **6** (from Method B)



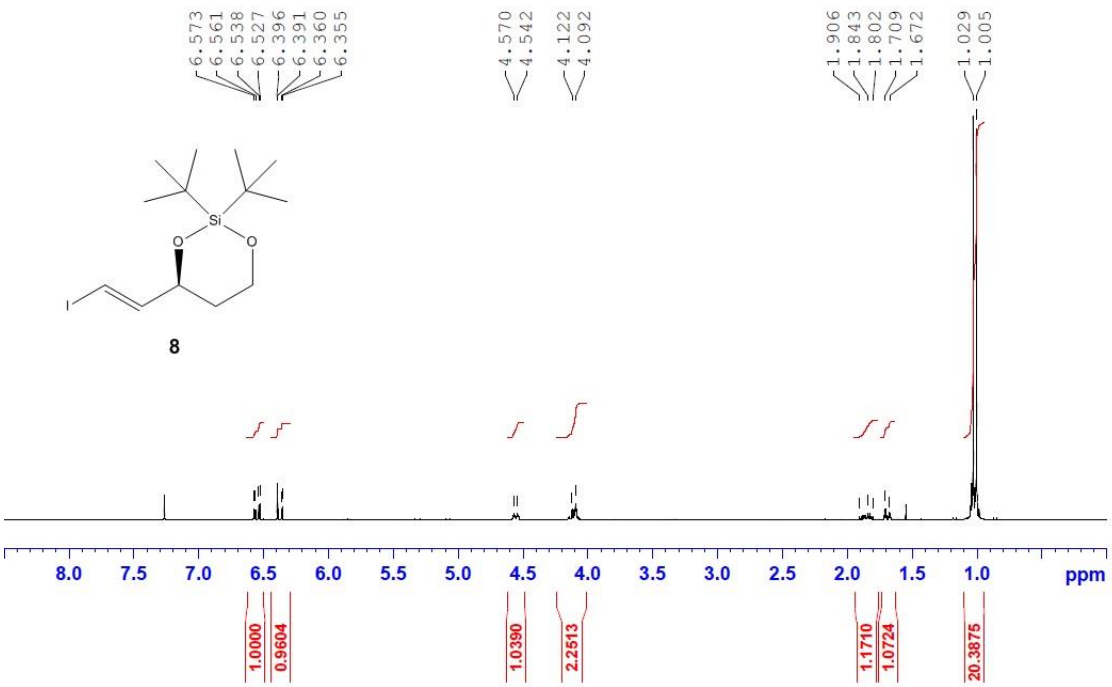


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **7**

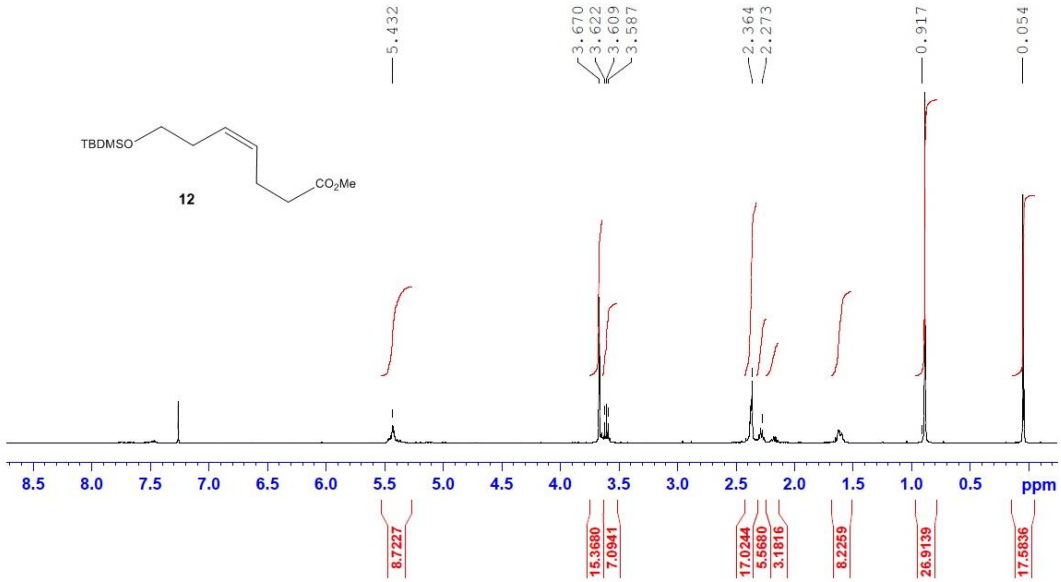




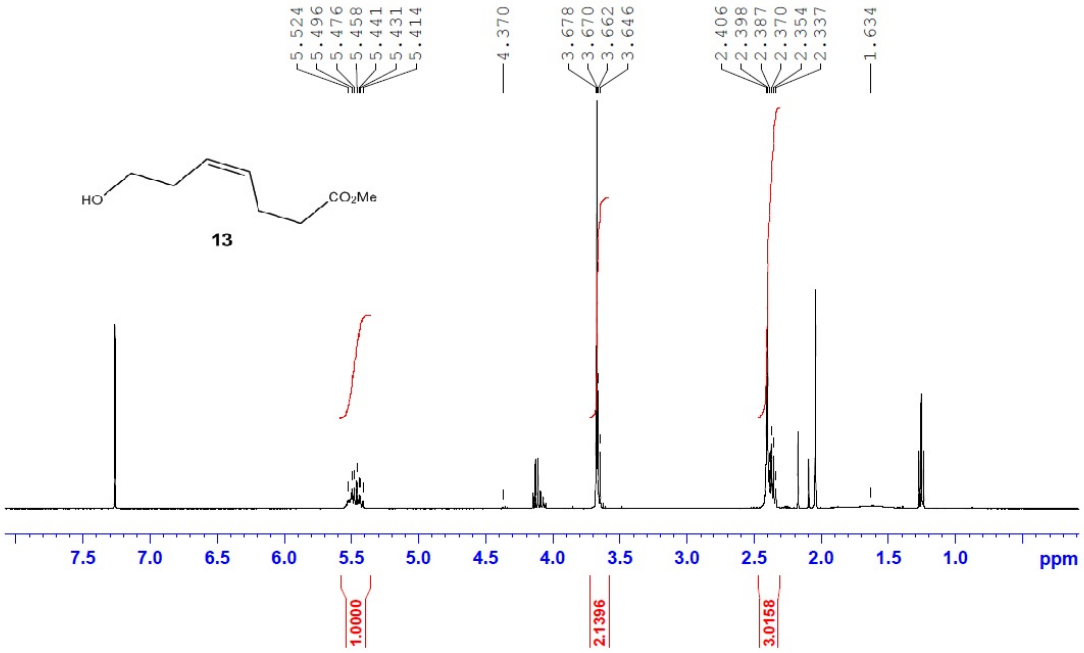
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8**



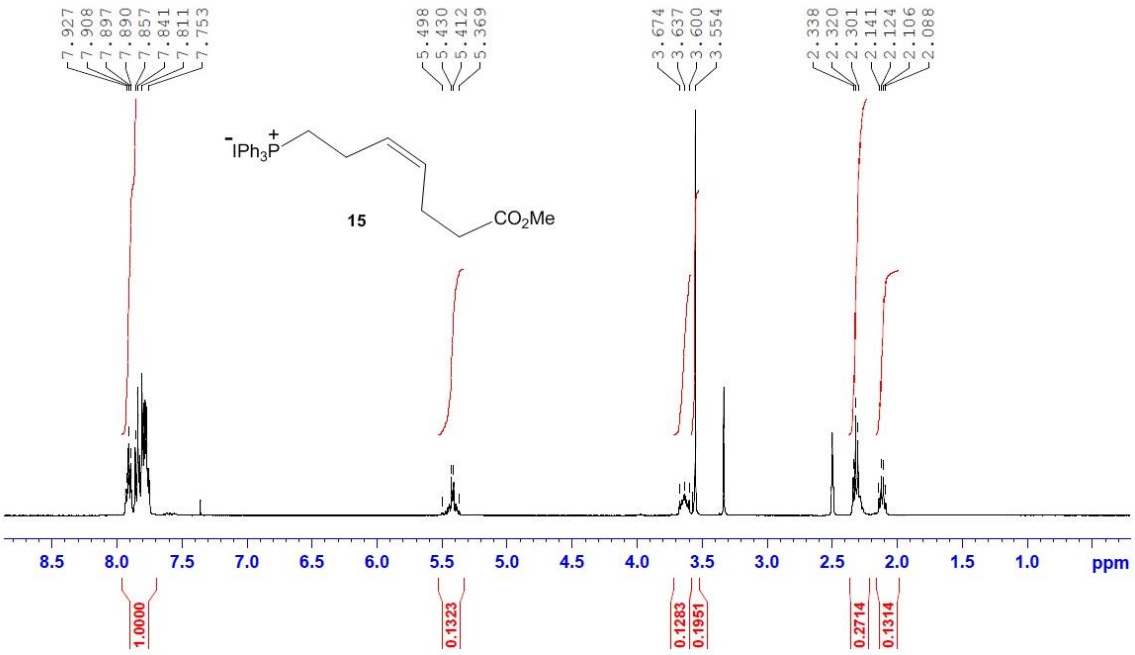
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **12**



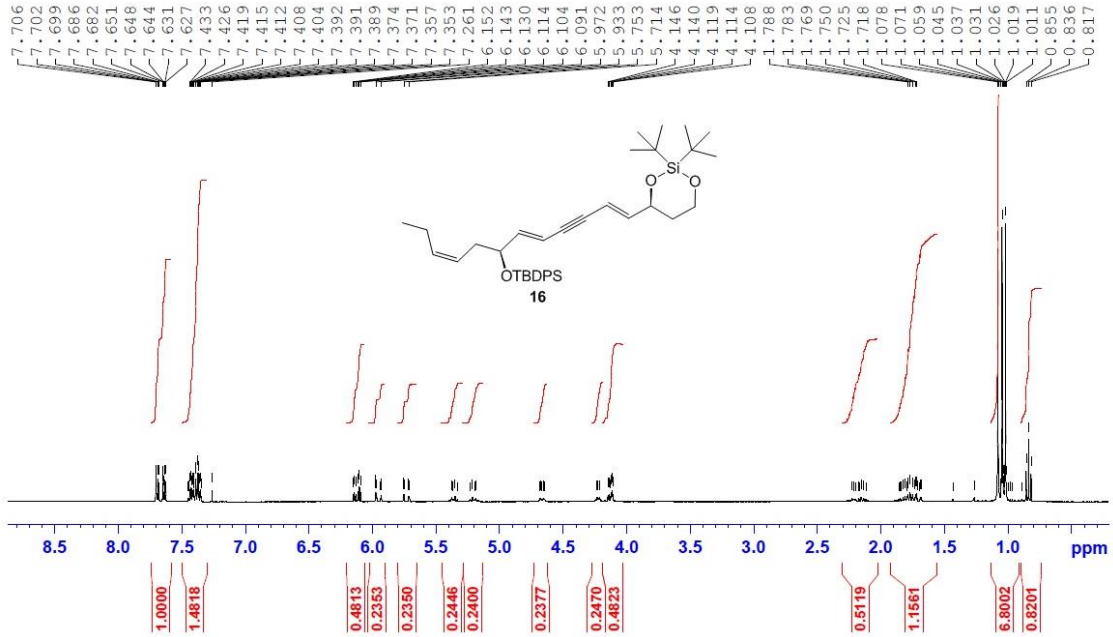
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **13**

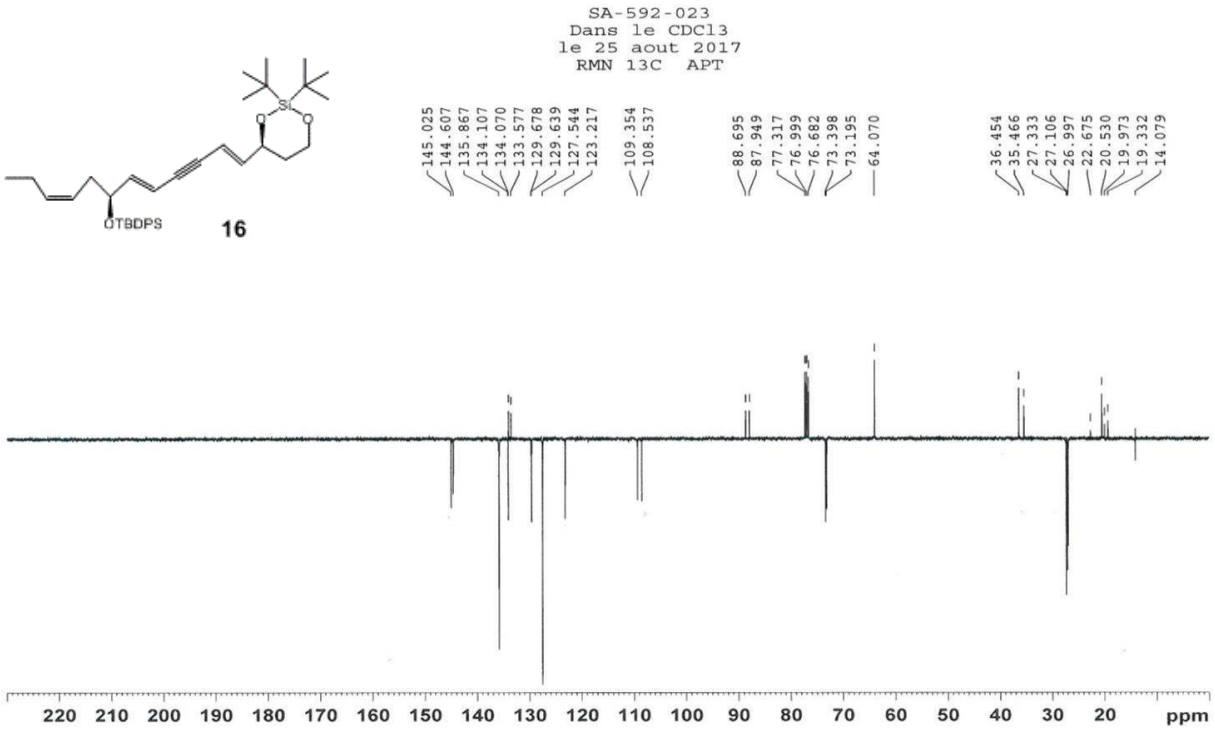


^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **15**

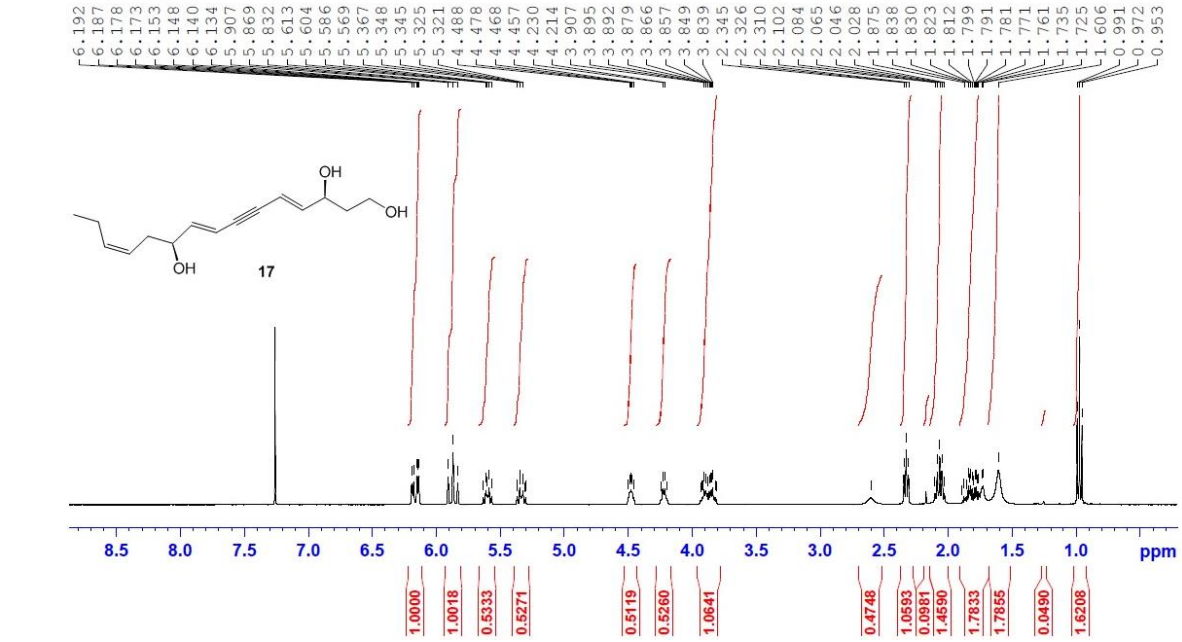


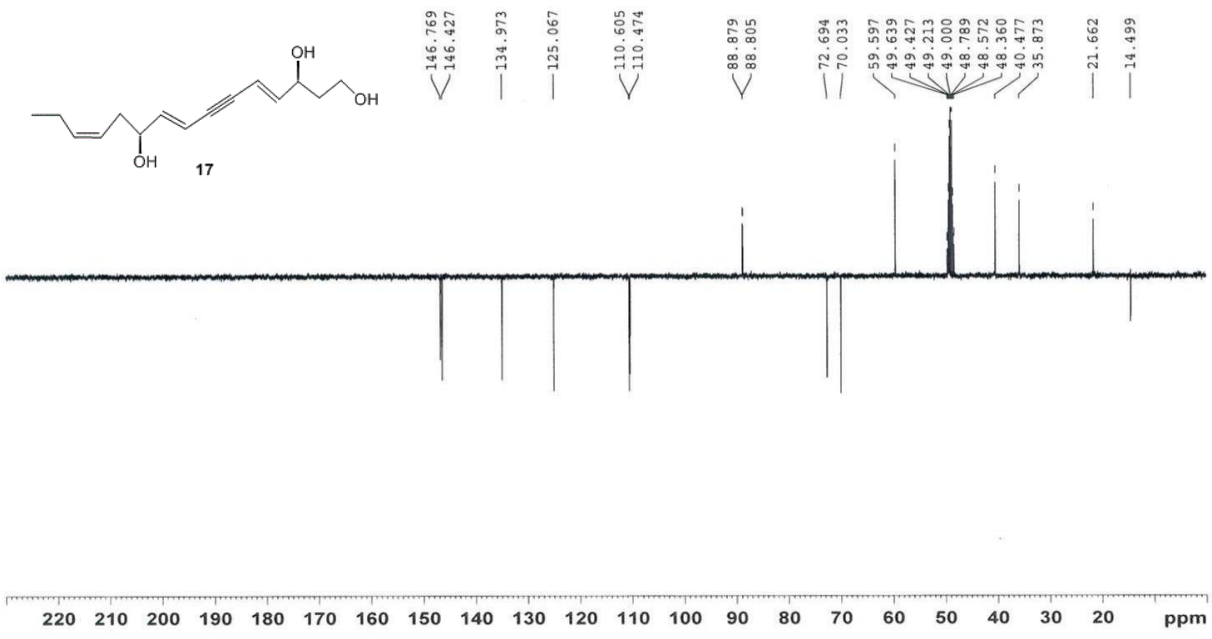
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **16**



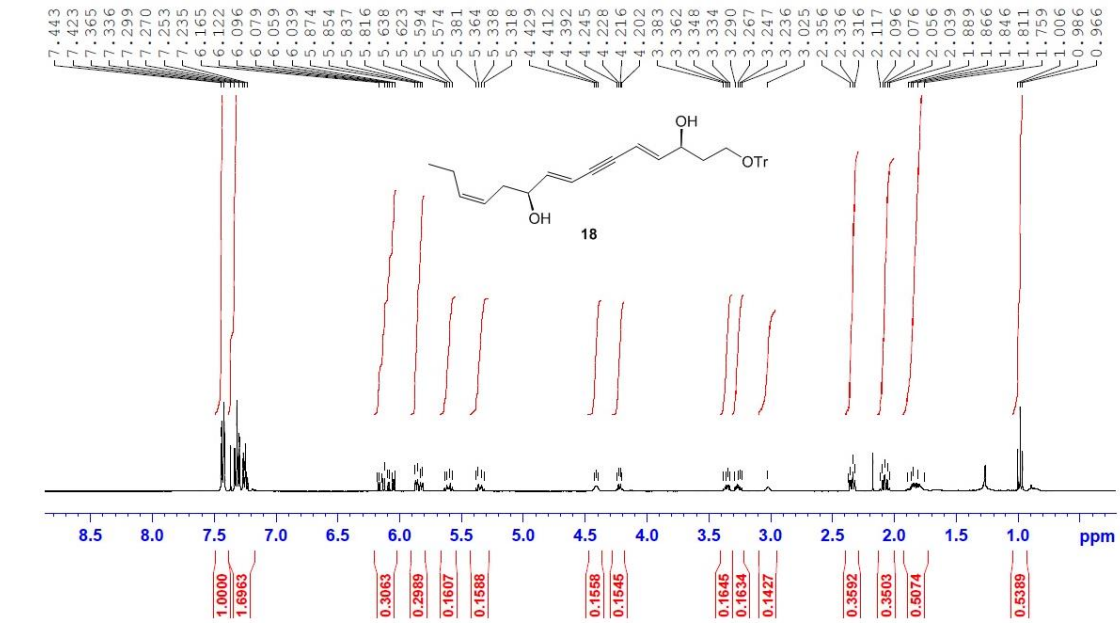


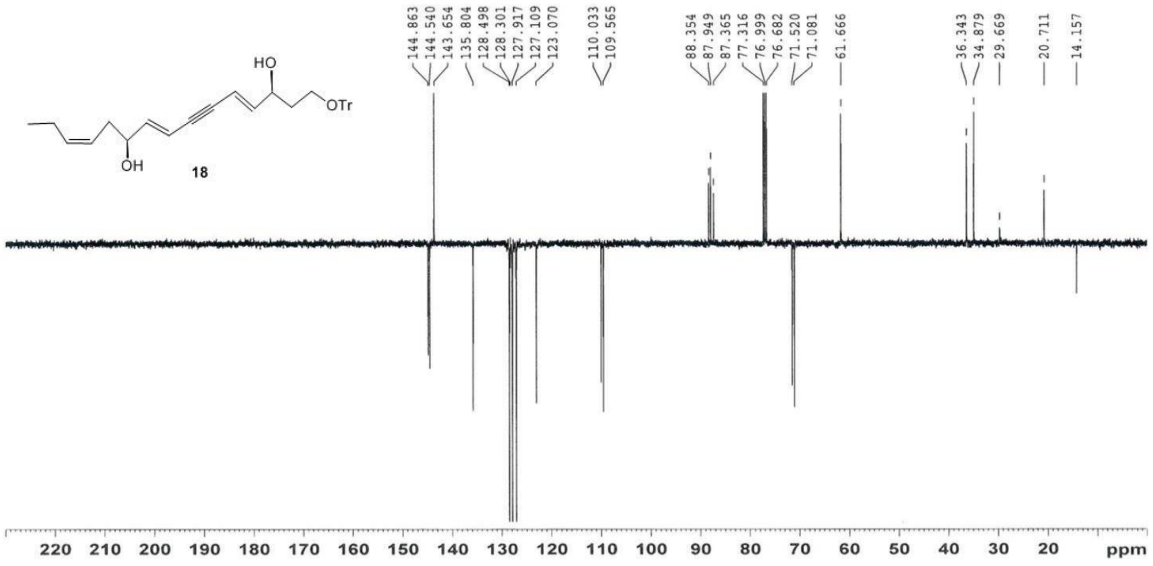
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, MeOH-d_4) spectra of **17**



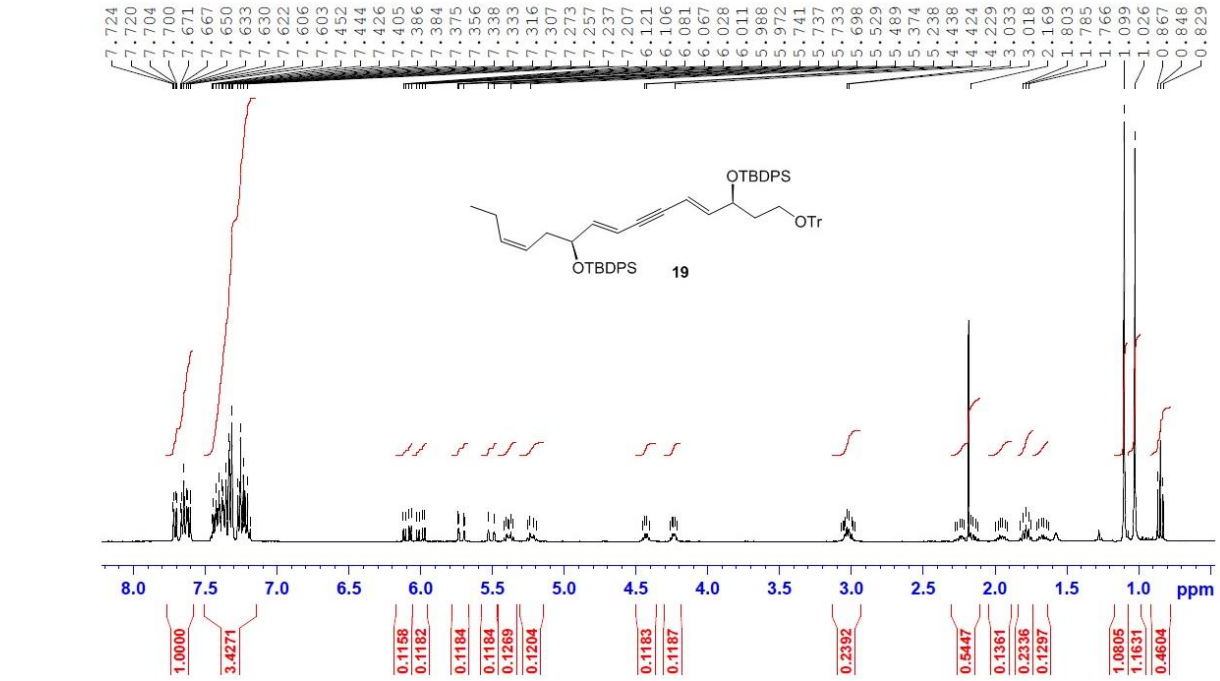


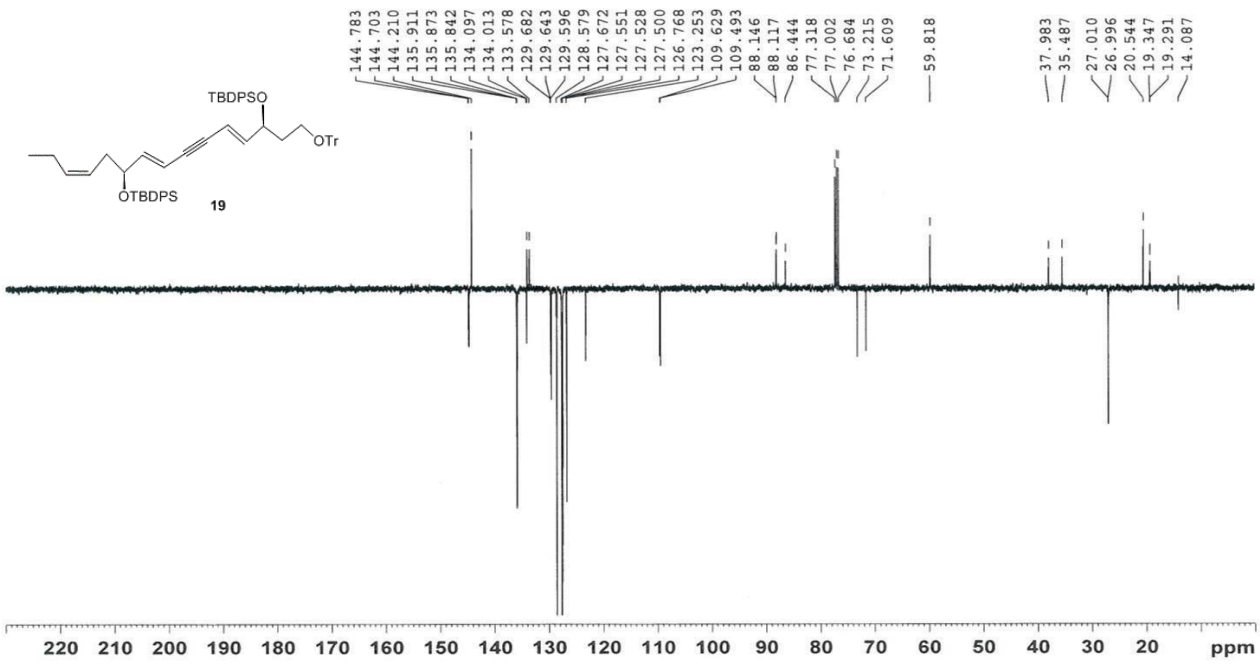
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **18**



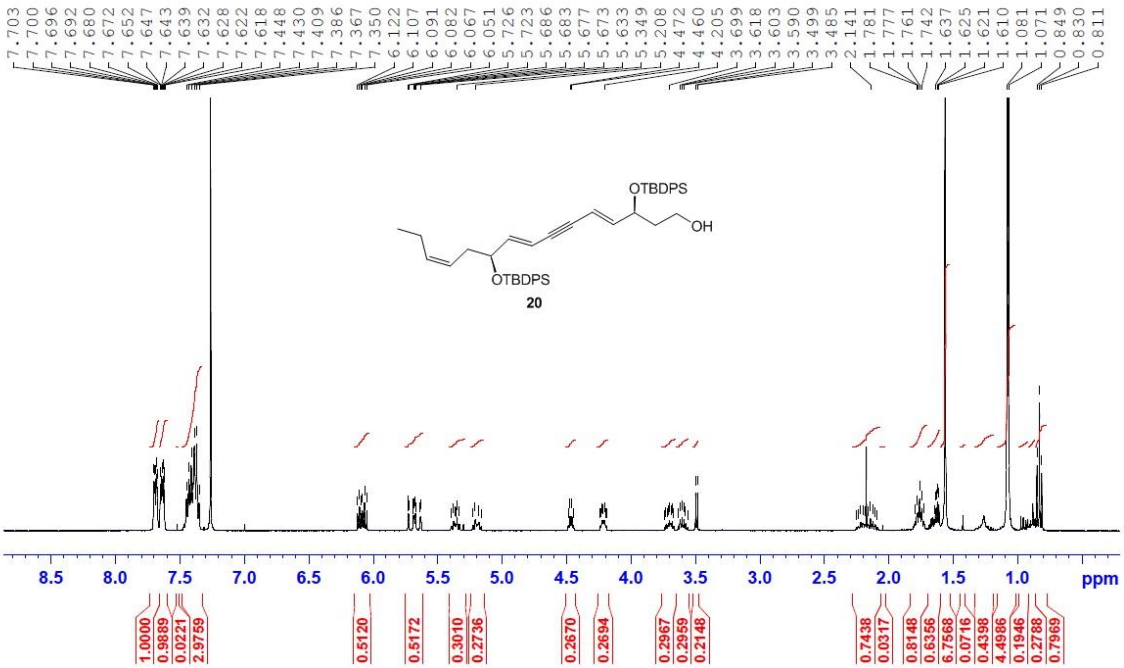


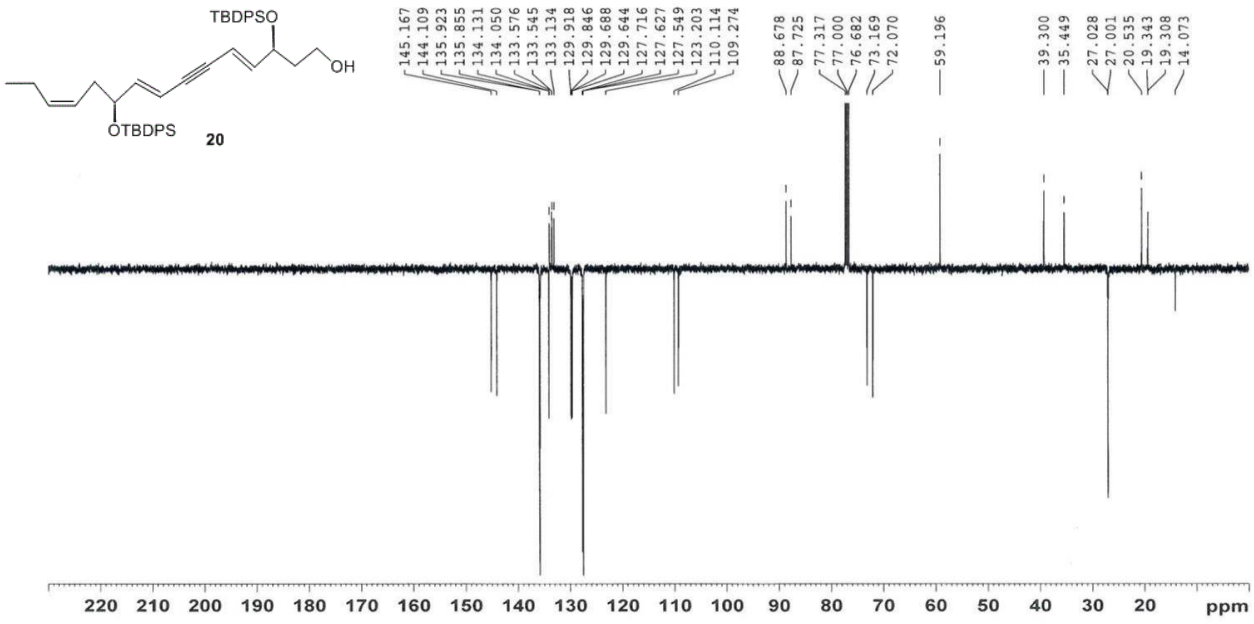
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **19**



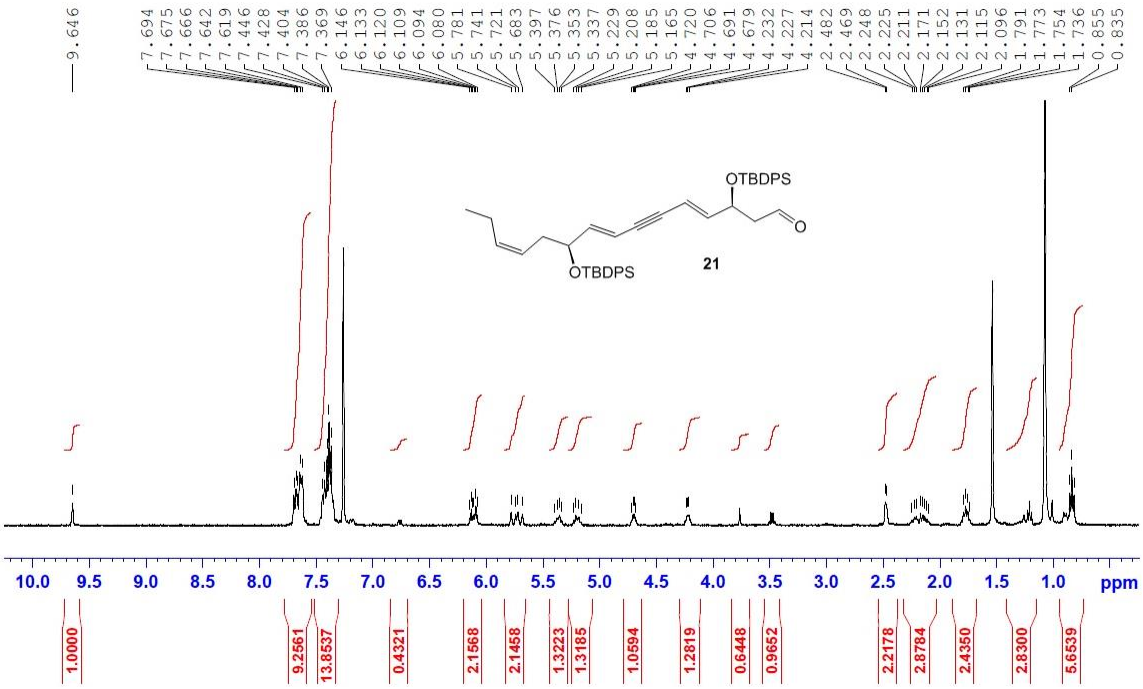


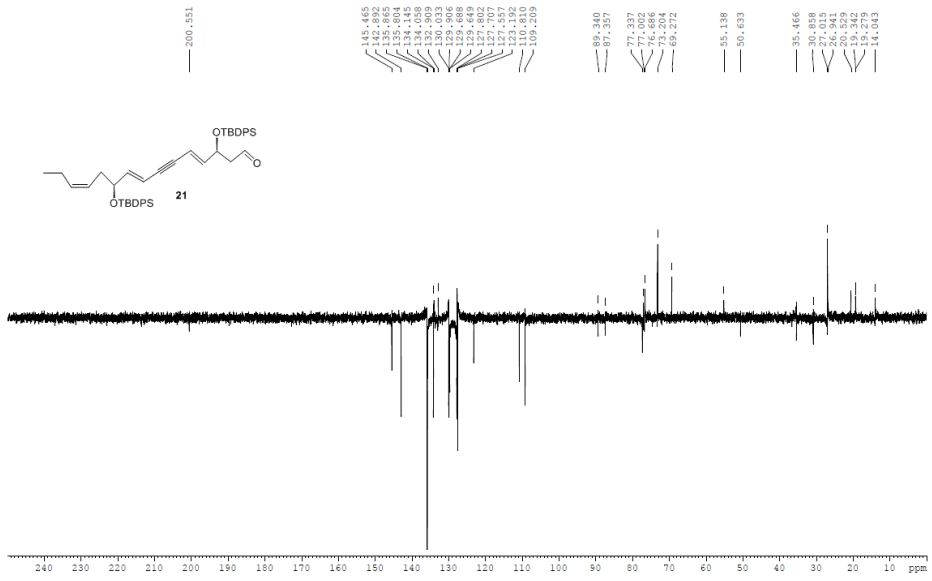
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **20**



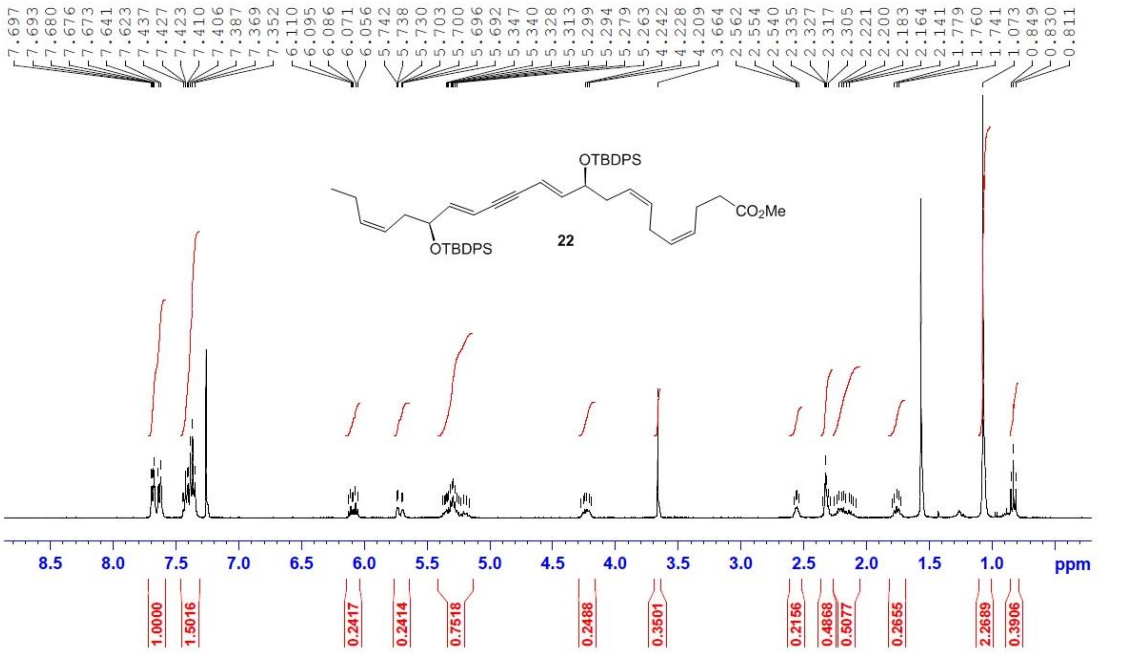


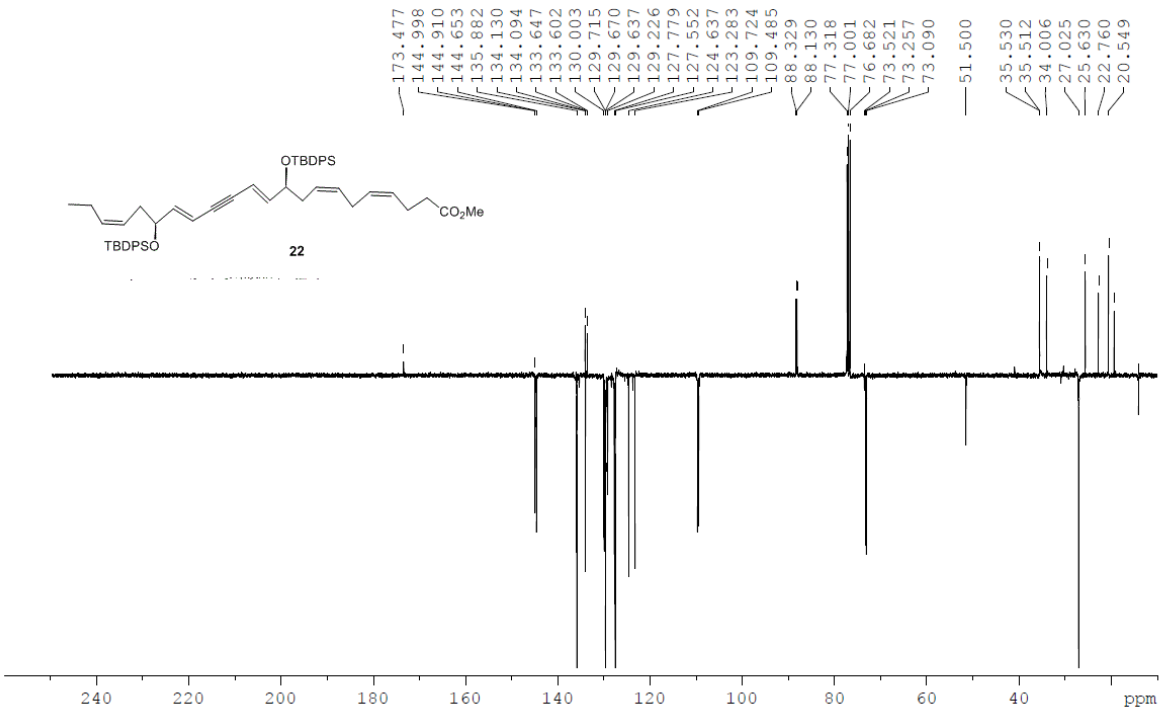
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **21**



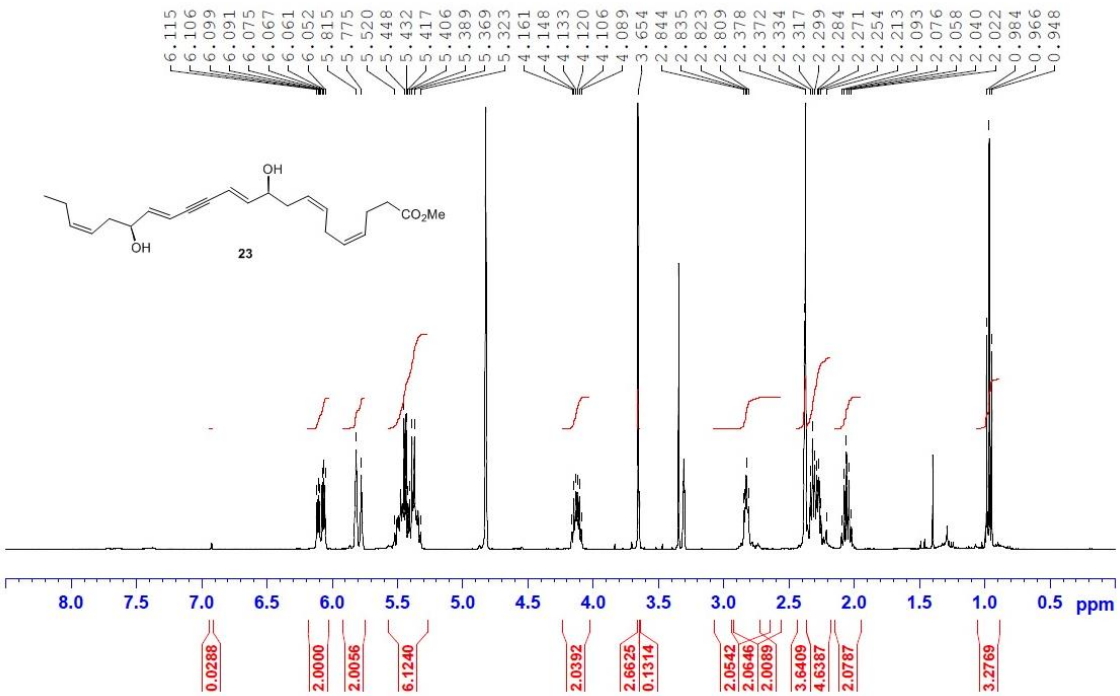


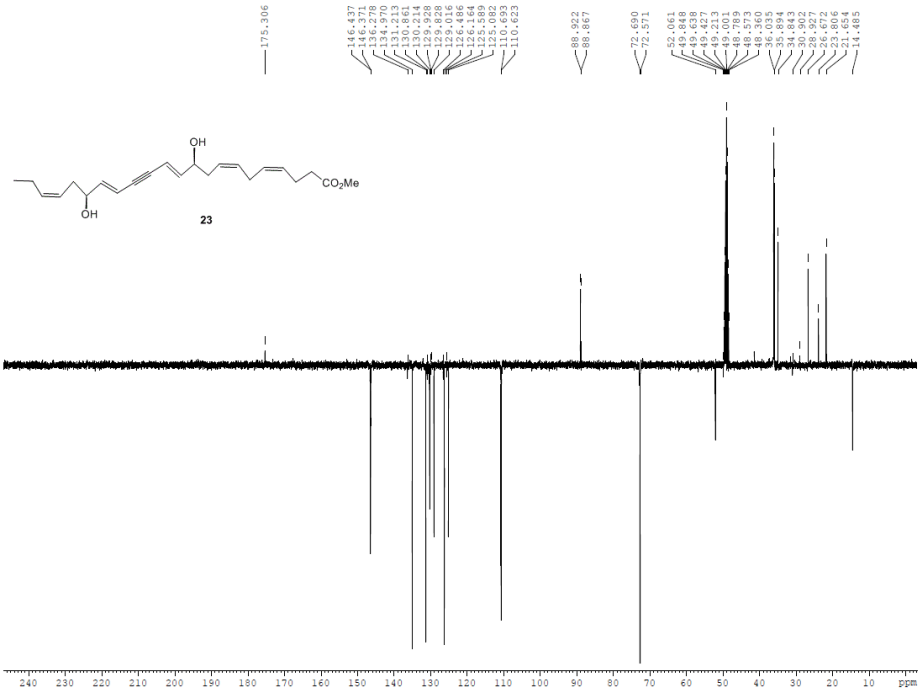
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR-APT (100 MHz, $CDCl_3$) spectra of **22**



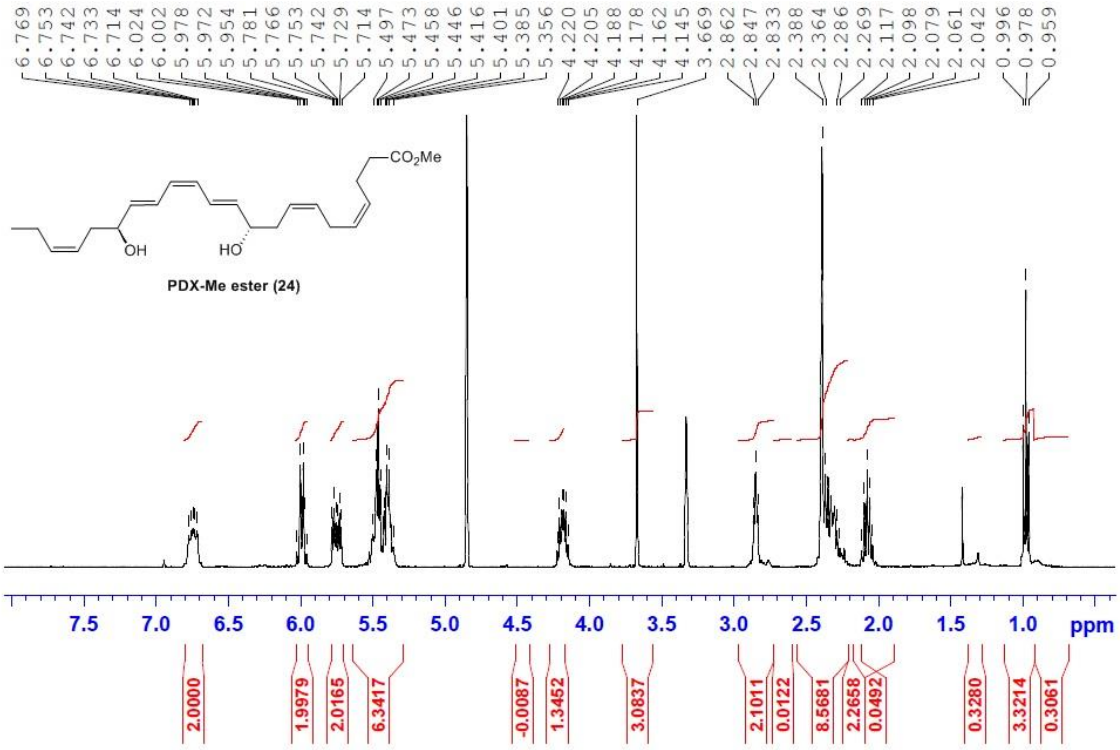


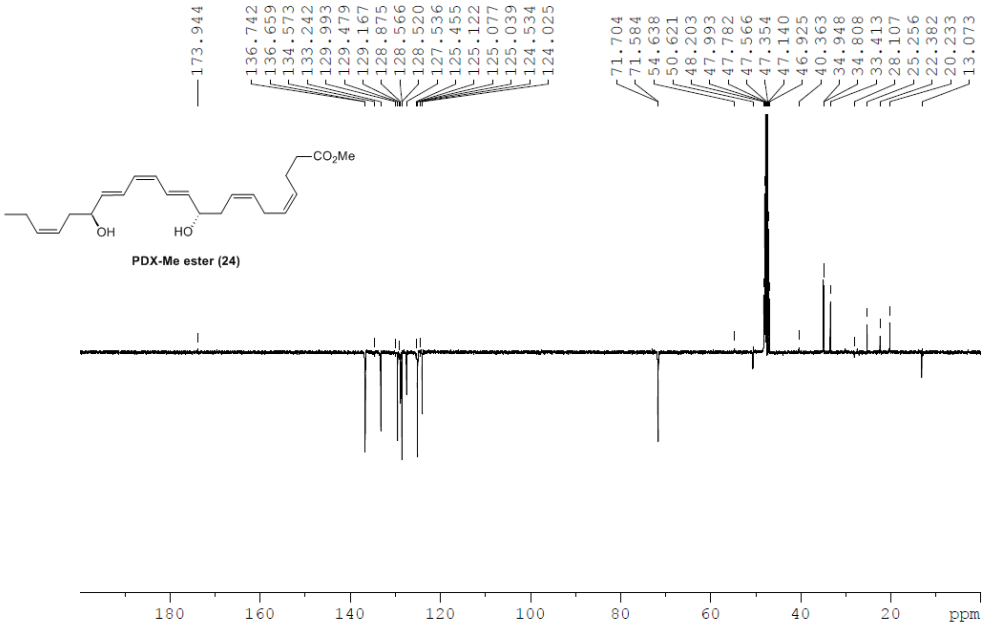
^{1}H NMR (400 MHz, MeOH-d_4) and ^{13}C NMR-APT (100 MHz, MeOH-d_4) spectra of spectrum of **23**



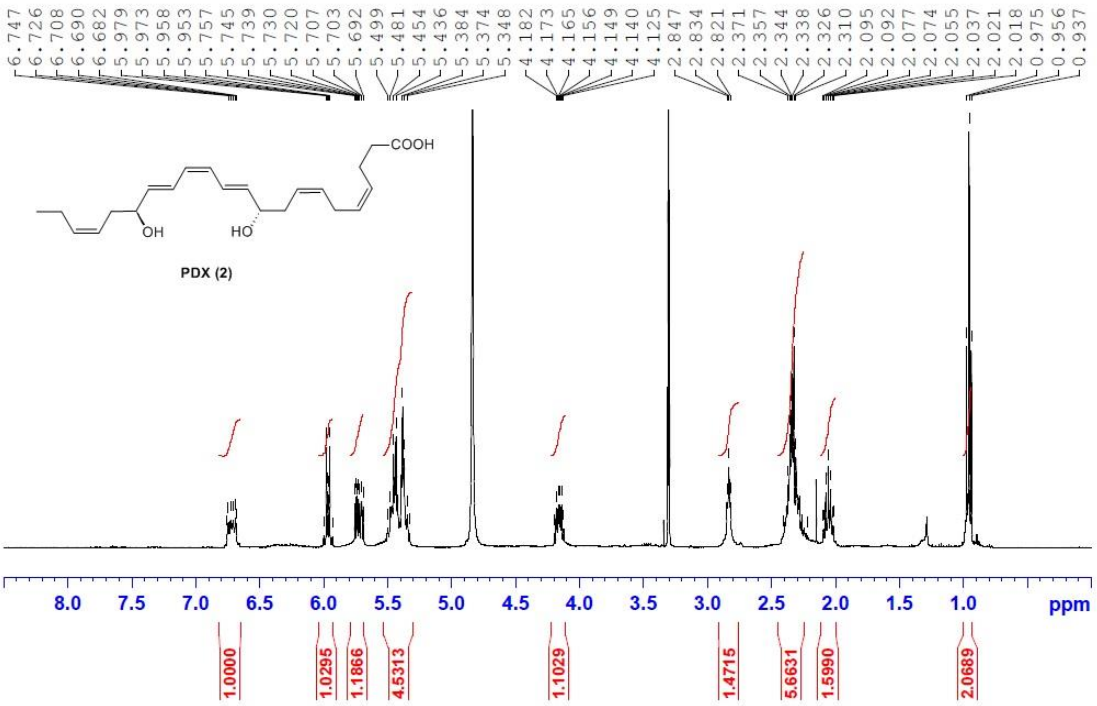


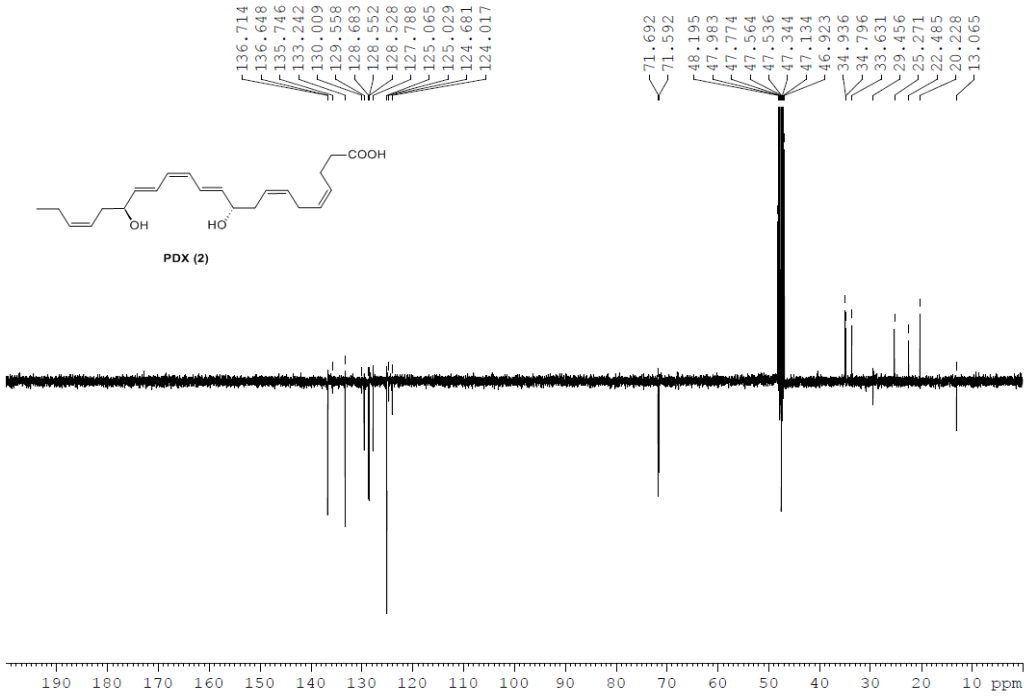
^{1}H NMR (400 MHz, MeOH-d_4) and ^{13}C NMR-APT (100 MHz, MeOH-d_4) spectra of (**24**)





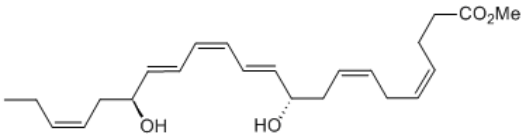
^{1}H NMR (400 MHz, MeOH-d_4) and ^{13}C NMR-APT (100 MHz, MeOH-d_4) spectra of PDX (**2**)



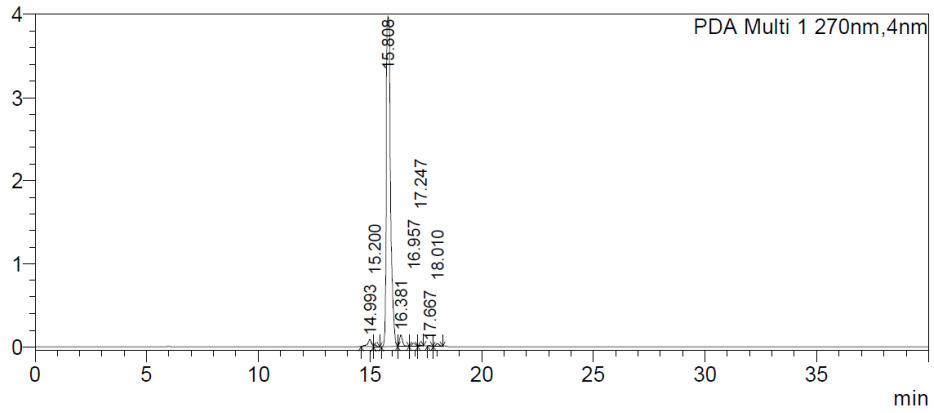


2.HPLC chromatograms of PDX-Me ester (**24**) and PDX (**2**)

HPLC (Altima C18 analytical reverse phase column, 270 nm) chromatogram of PDX-Me ester (**24**)



PDX-Me ester (24)

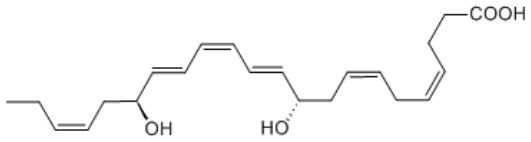


Peak Table

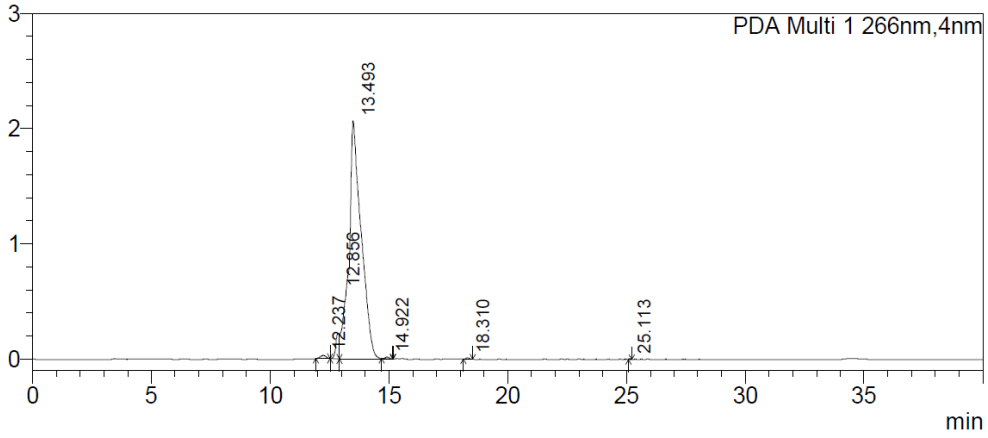
PDA Ch1 270nm

Peak#	Ret. Time	Area	Area%
1	14.993	1059678	1.901
2	15.200	191351	0.343
3	15.808	52230678	93.677
4	16.381	1328387	2.382
5	16.957	412084	0.739
6	17.247	95976	0.172
7	17.667	55298	0.099
8	18.010	382700	0.686
Total		55756153	100.000

HPLC (Altima C18 analytical reverse phase column, 266nm) chromatogram of PDX (**2**)



PDX (2)



Peak Table

PDA Ch1 266nm

Peak#	Ret. Time	Area	Area%
1	12.237	489162	0.629
2	12.856	2282127	2.935
3	13.493	74673982	96.053
4	14.922	150946	0.194
5	18.310	127524	0.164
6	25.113	18756	0.024
Total		77742497	100.000

3-UV-vis absorption spectrum (in MeOH from HPLC-PDA detection) of PDX (**2**)