Supplementary data

Dokdolipids A−C, Hydroxylated Rhamnolipids from the Marine-Derived Actinomycete *Actinoalloteichus hymeniacidonis*

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Contents

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
82 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-40 H: 1-60 O: 1-20 Na: 1-1

Minimum:				-1.5				
Maximum:		100.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
485.3094	485.3090	0.4	0.8	1.5	683.2	n/a	n/a	C24 H46 O8 Na

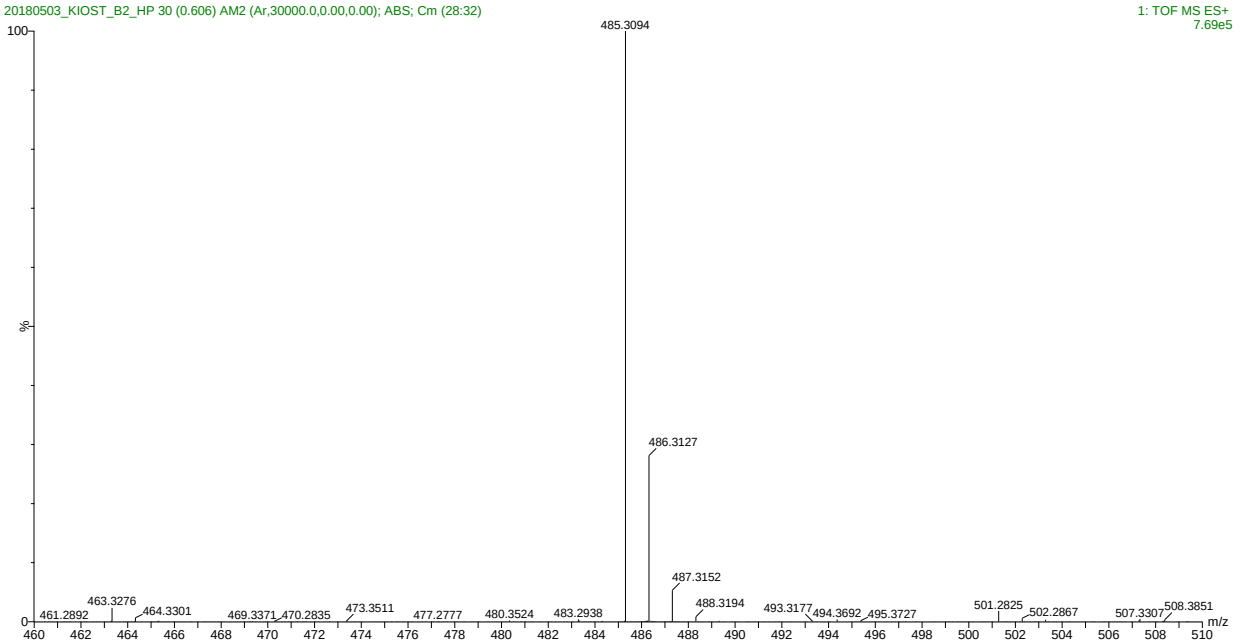

Figure S1. HRESIMS data of dokdolipid A (**1**).

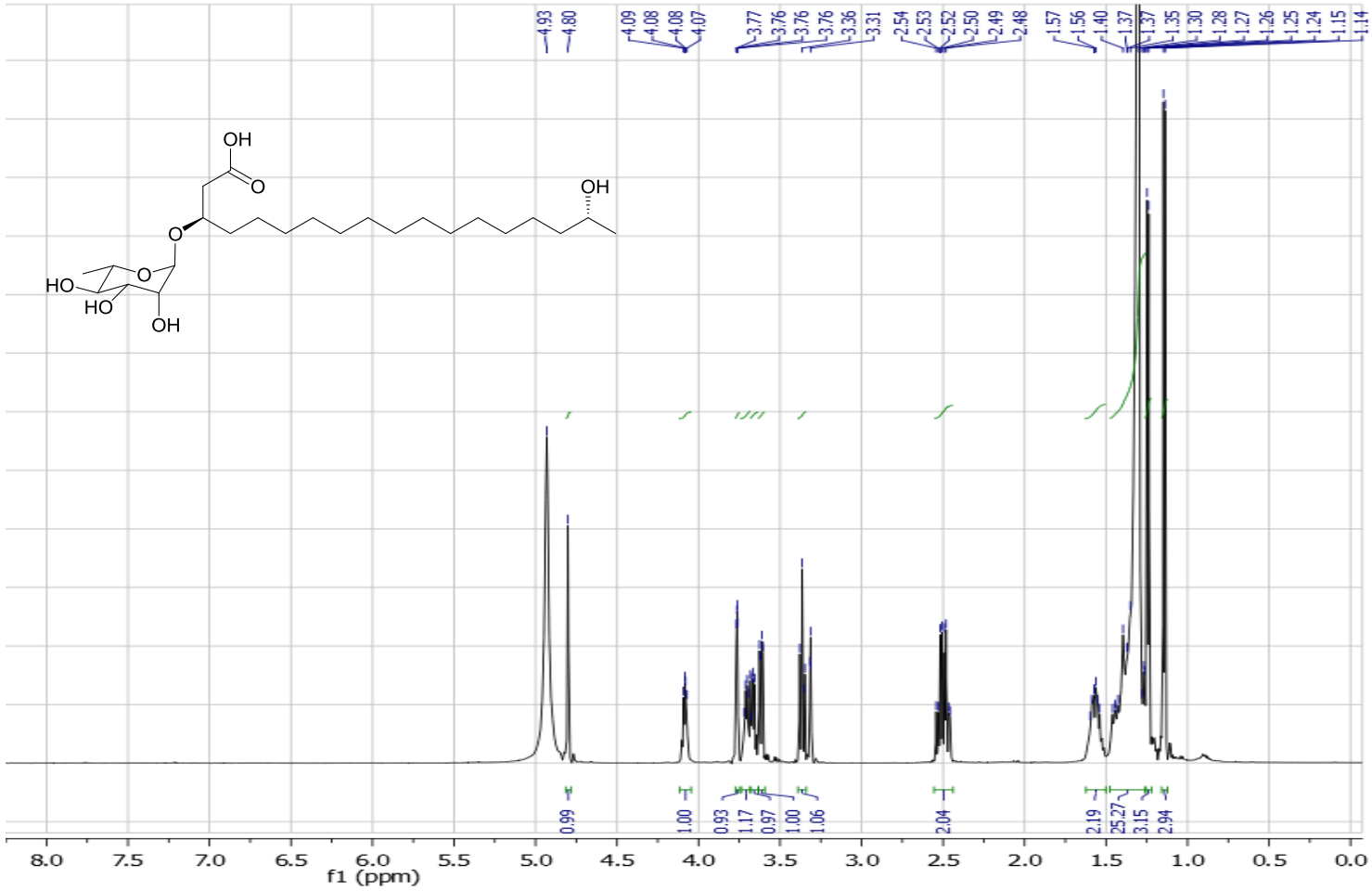

Figure S2. ^{1}H NMR spectrum of dokdolipid A (**1**).

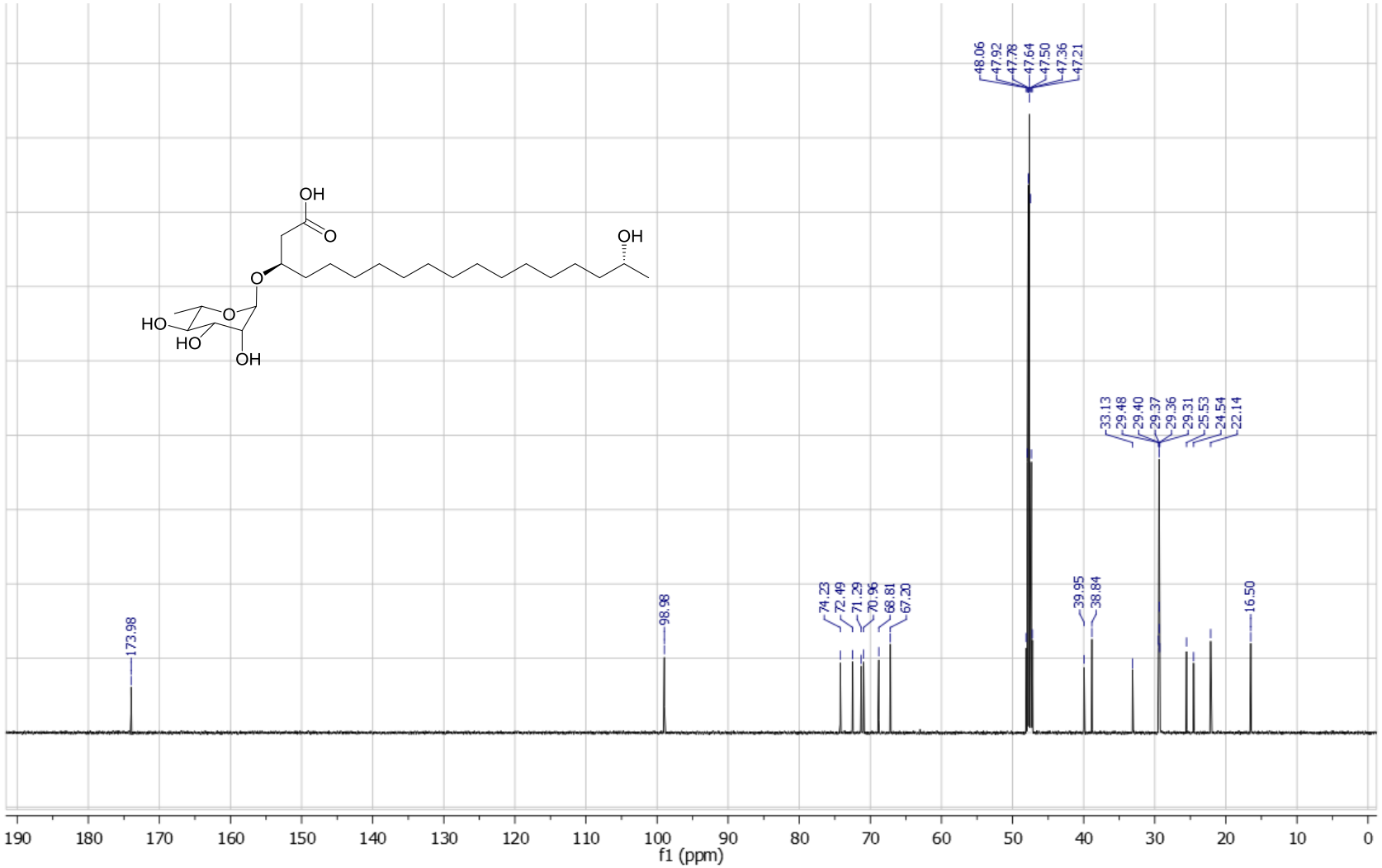

Figure S3. ^{13}C NMR spectrum of dokdolipid A (**1**).

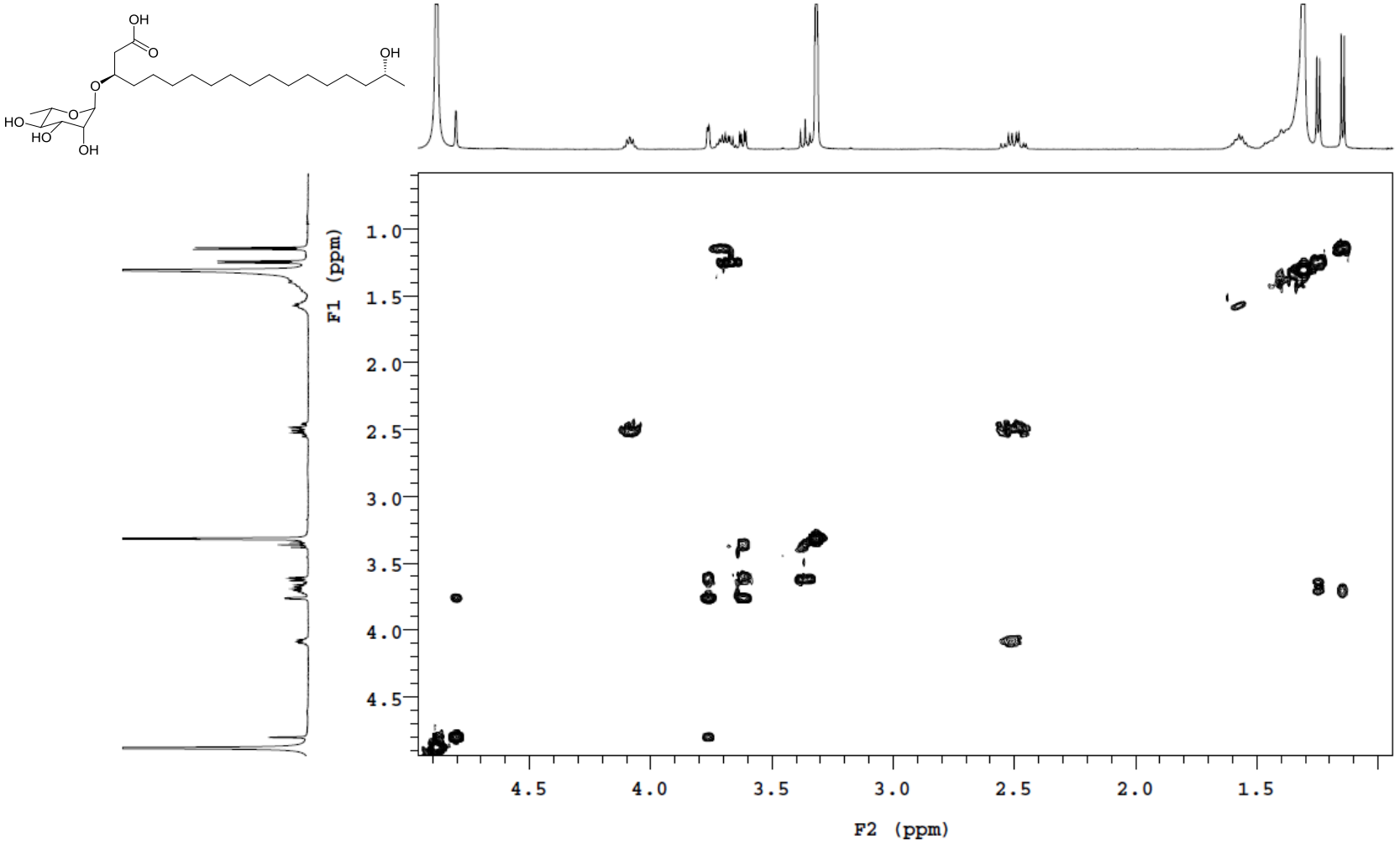

Figure S4. ^{1}H-^{1}H COSY spectrum of dokdolipid A (**1**).

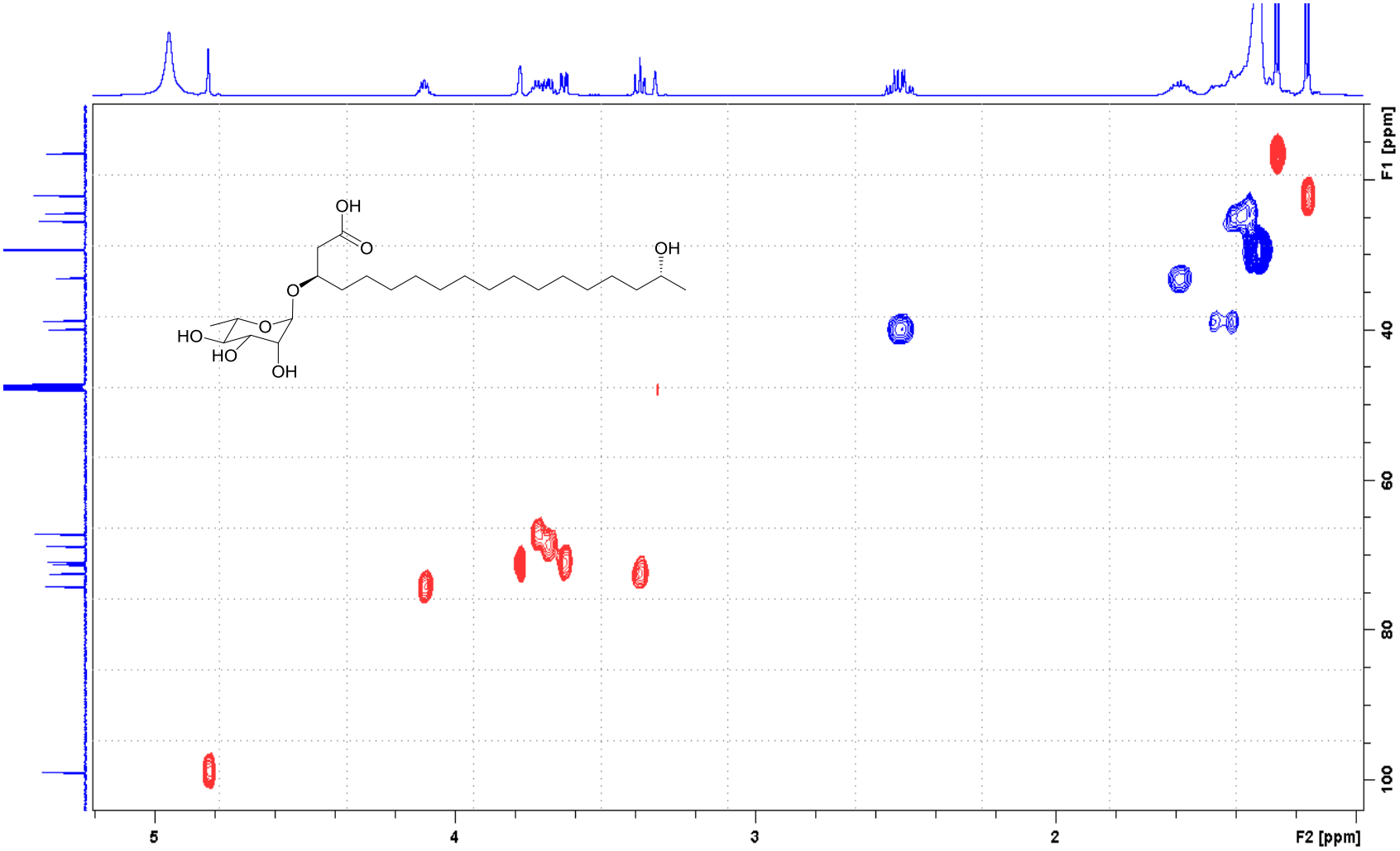

Figure S5. HSQC spectrum of dokdolipid A (**1**).

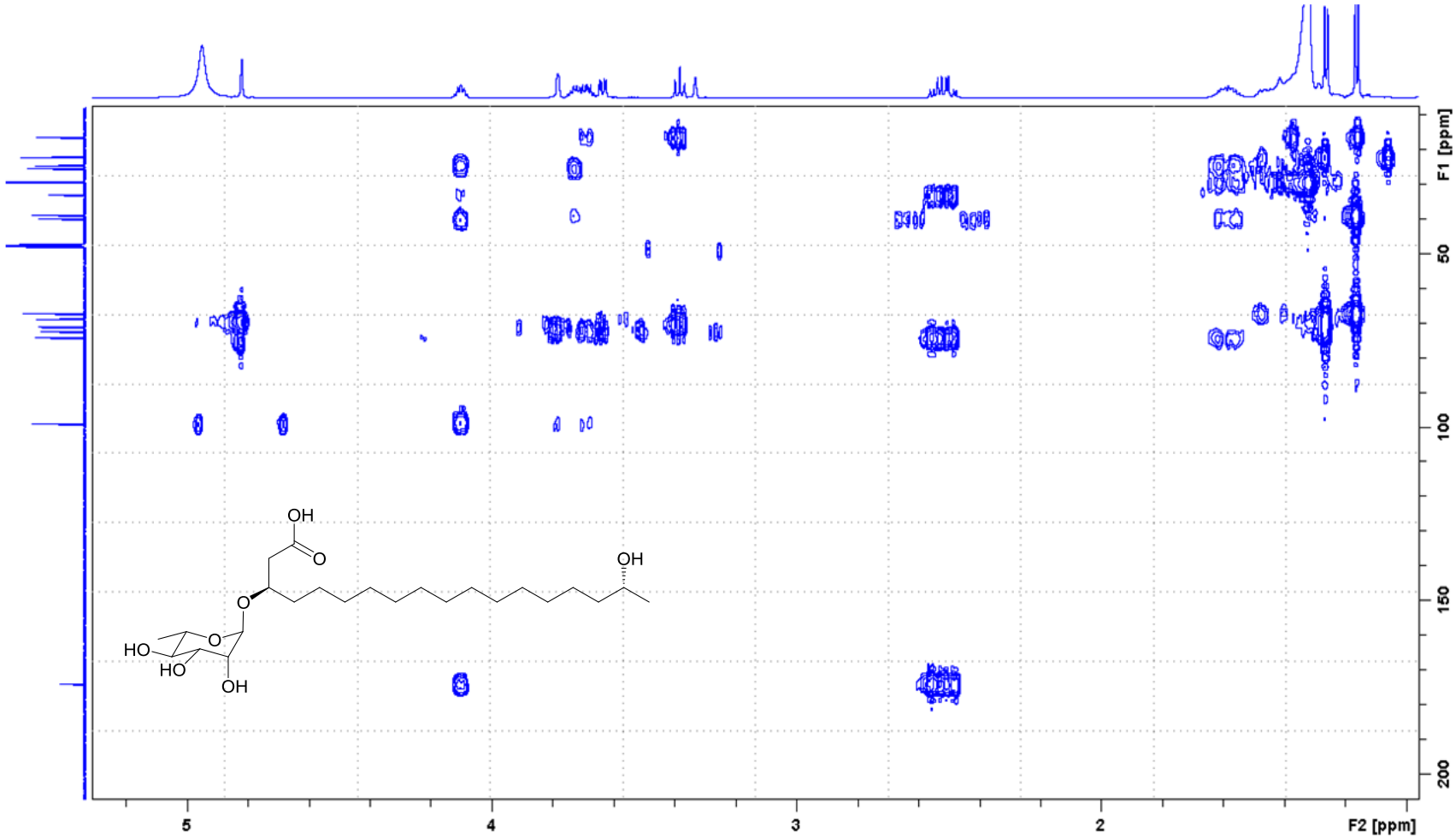

Figure S6. HMBC spectrum of dokdolipid A (**1**).

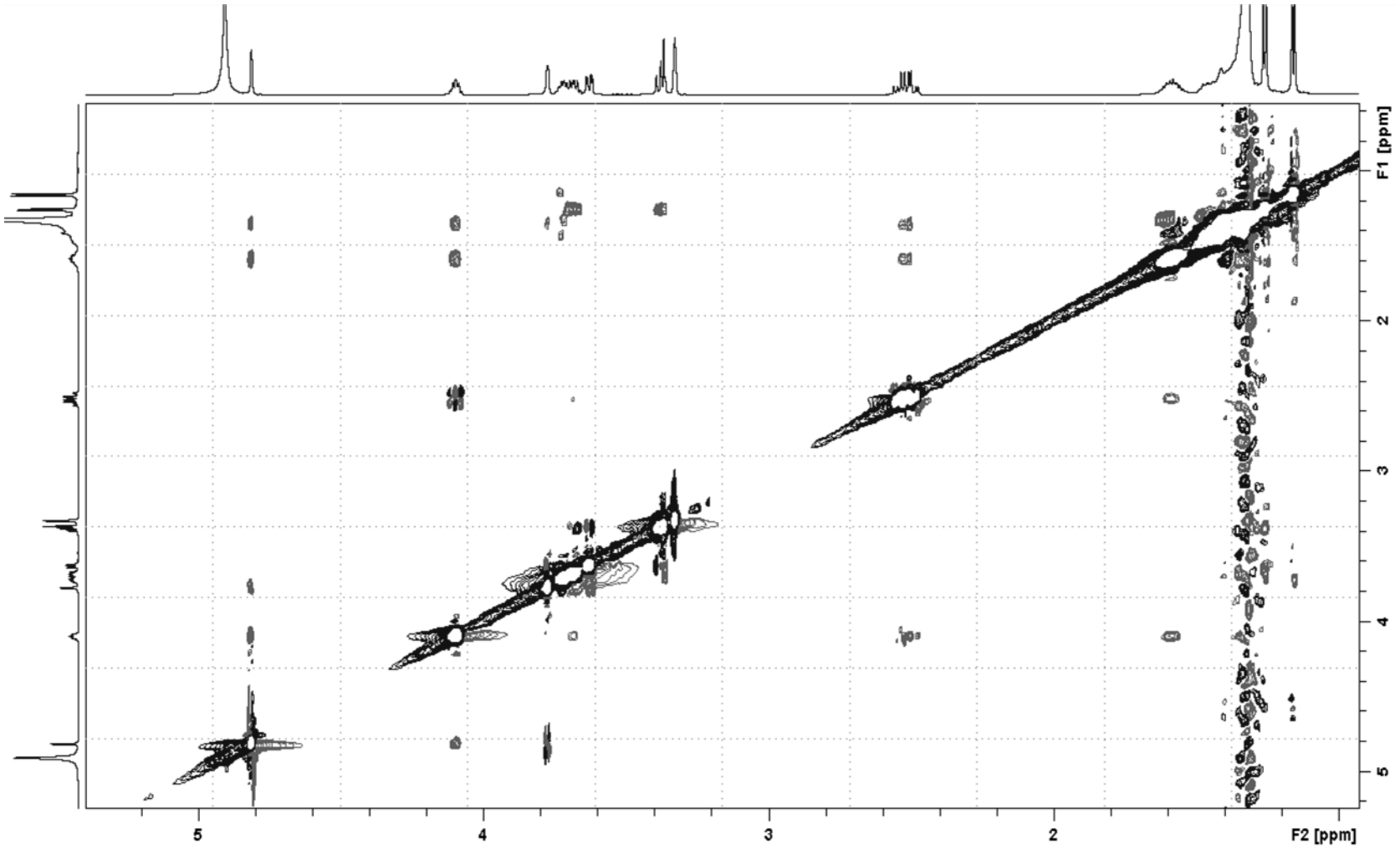

Figure S7. ROESY spectrum of dokdolipid A (**1**).

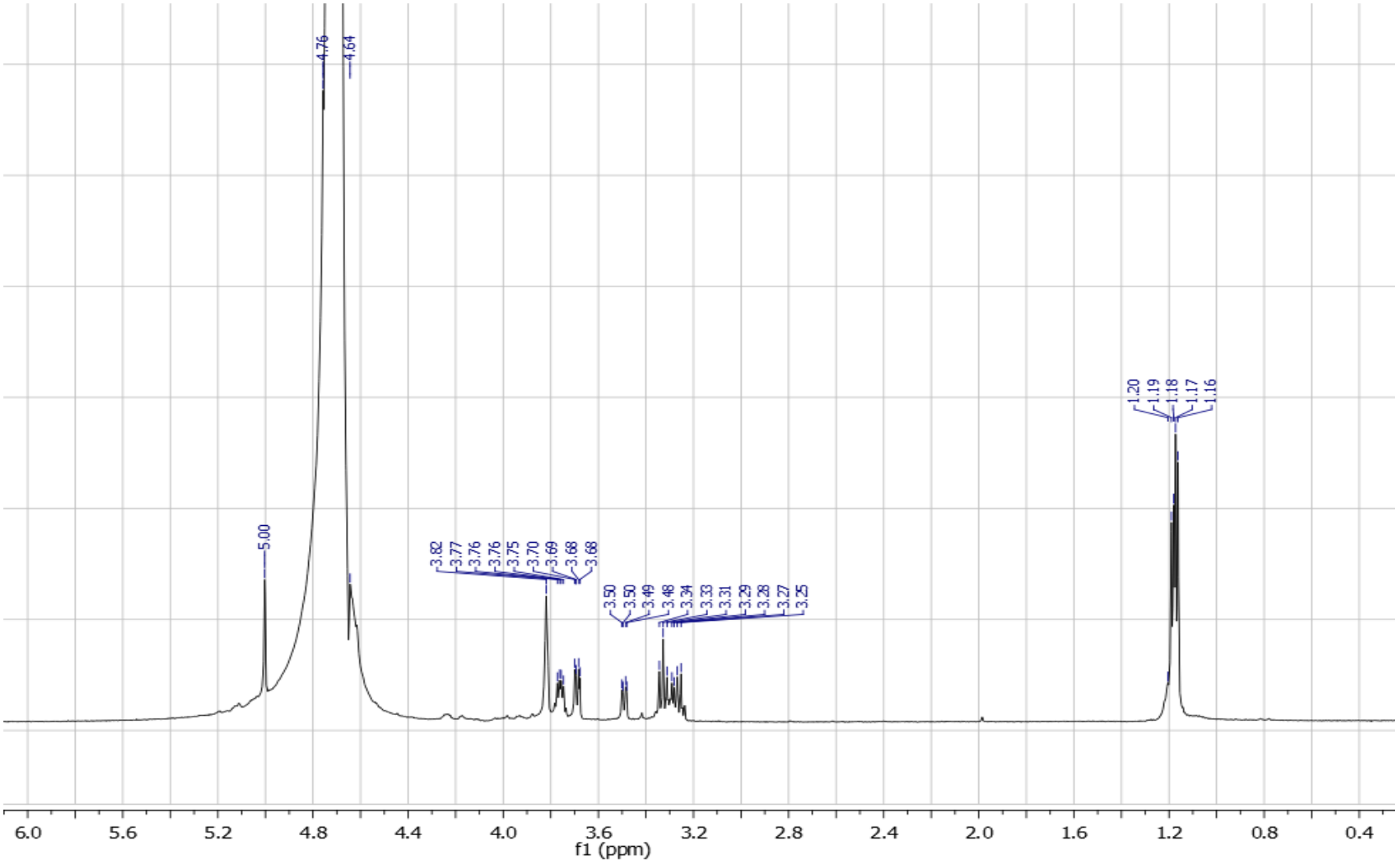

Figure S8. ^{1}H NMR spectrum of the hydrolysate of dokdolipid A (**1**).

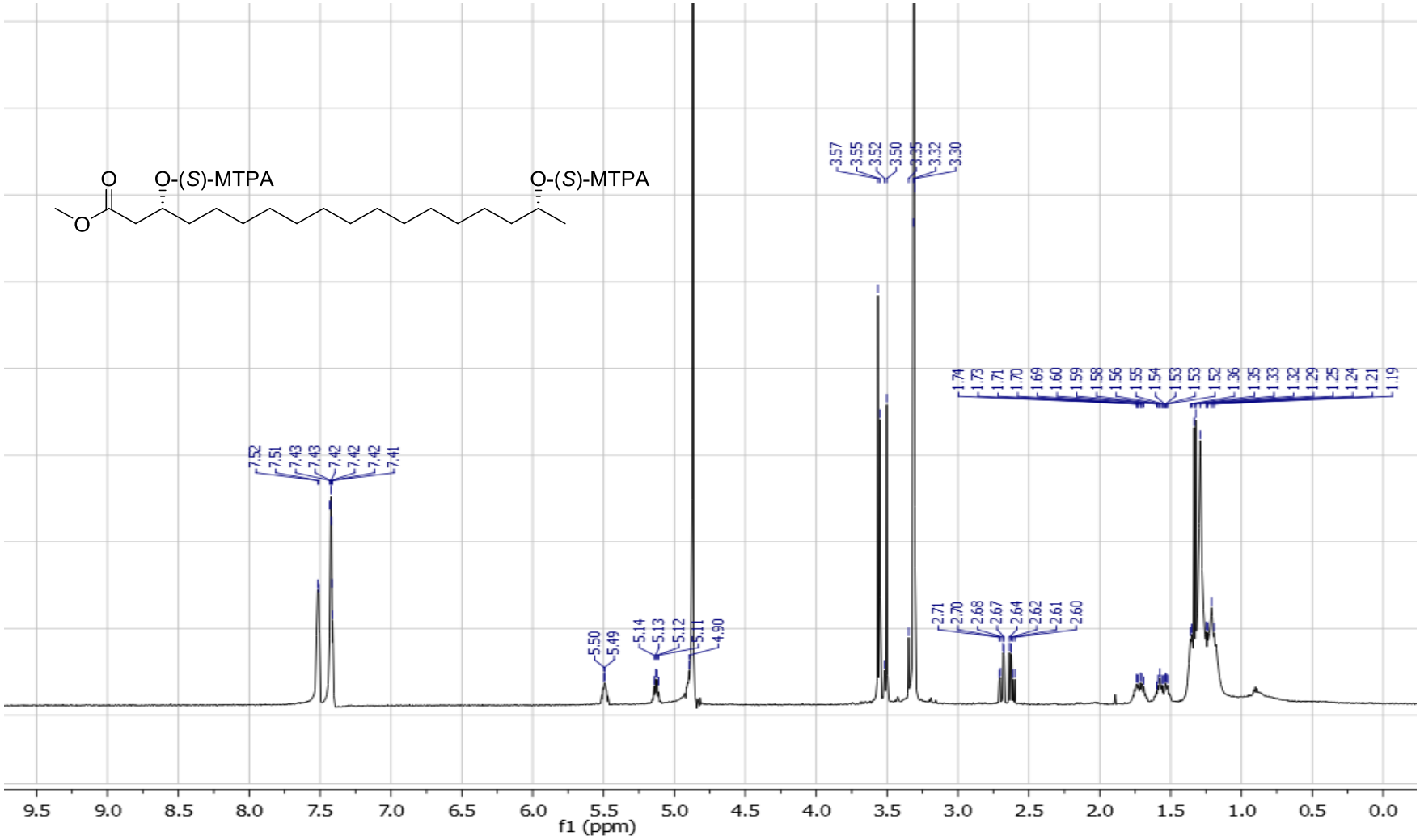

Figure S9. ^{1}H NMR spectrum of (*S*)-MTPA (**1a**) ester.

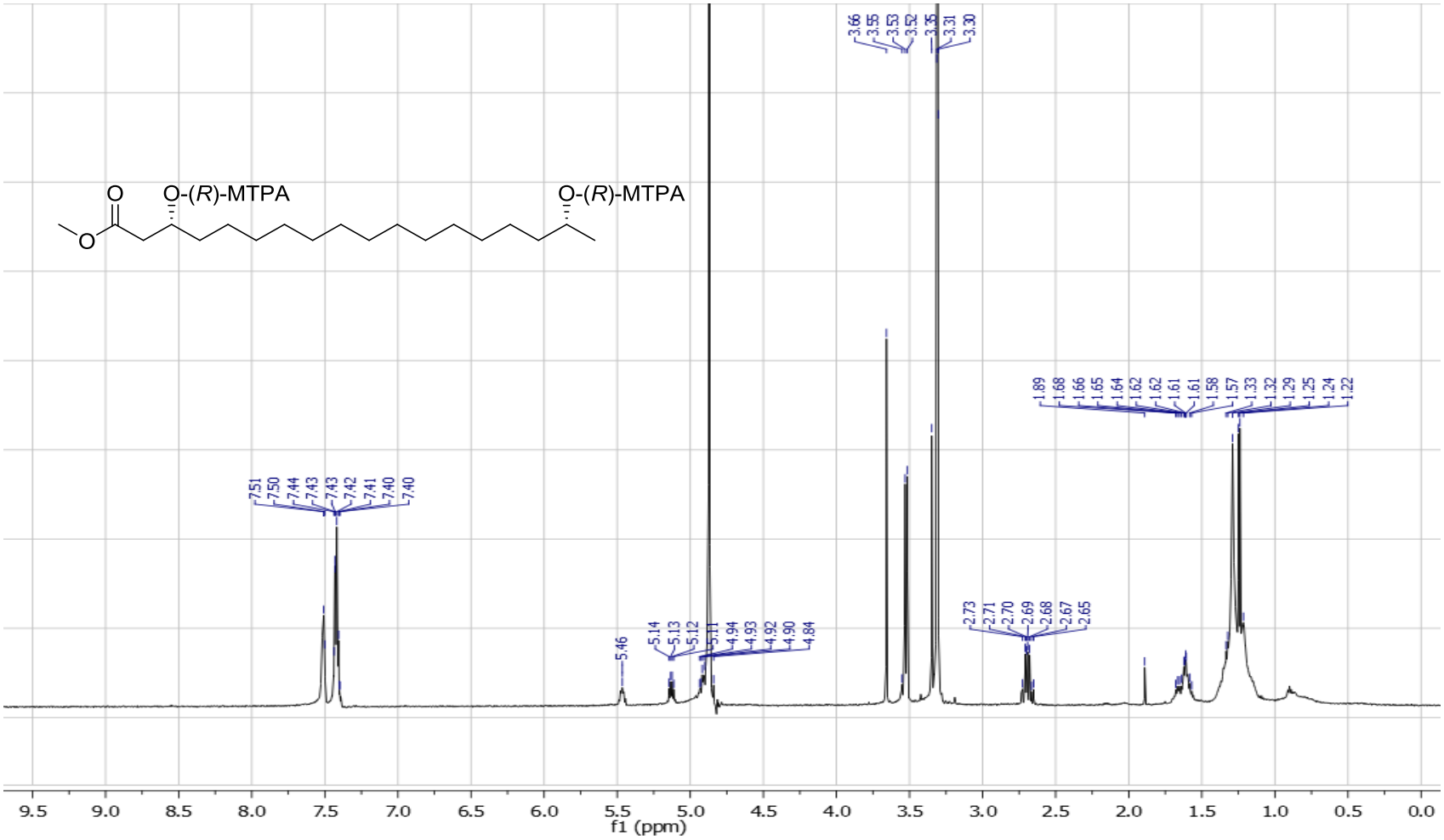

Figure S10. ^{1}H NMR spectrum of (*R*)-MTPA (**1b**) ester.

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Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
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Monoisotopic Mass, Even Electron Ions
79 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-40 H: 1-60 O: 1-20 Na: 1-1

Minimum:				-1.5				
Maximum:		100.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
483.2936	483.2934	0.2	0.4	2.5	686.0	n/a	n/a	C24 H44 O8 Na

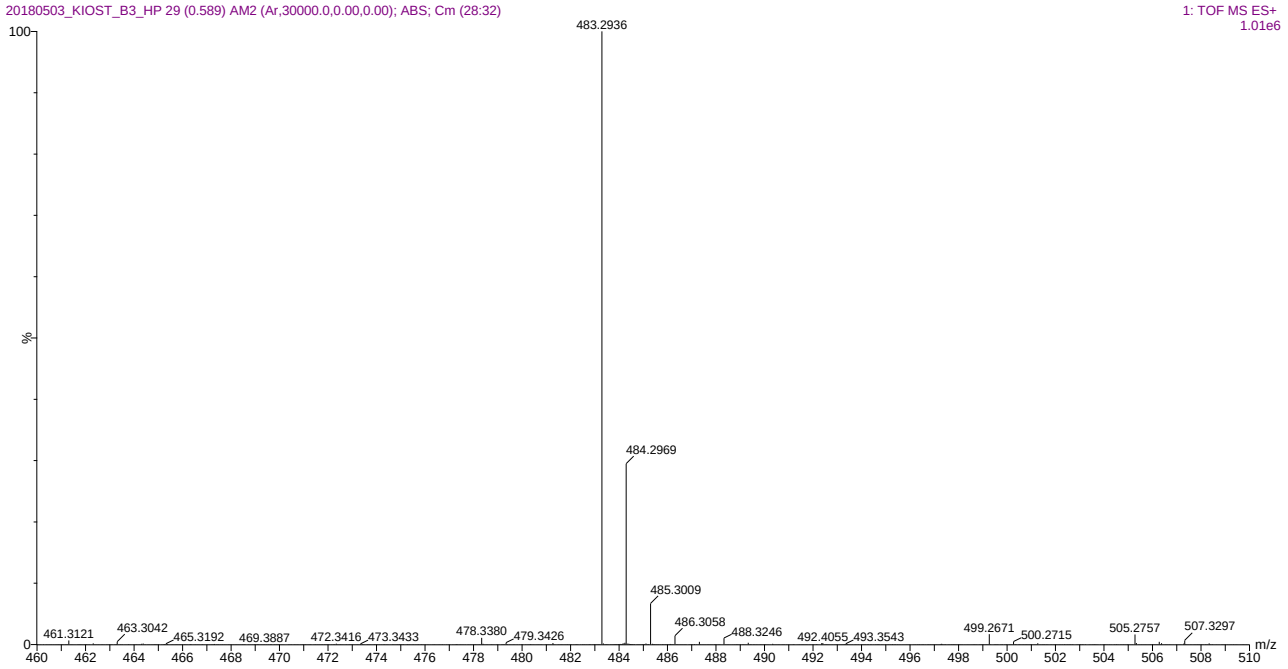

Figure S11. HRESIMS data of dokdolipid B (**2**).

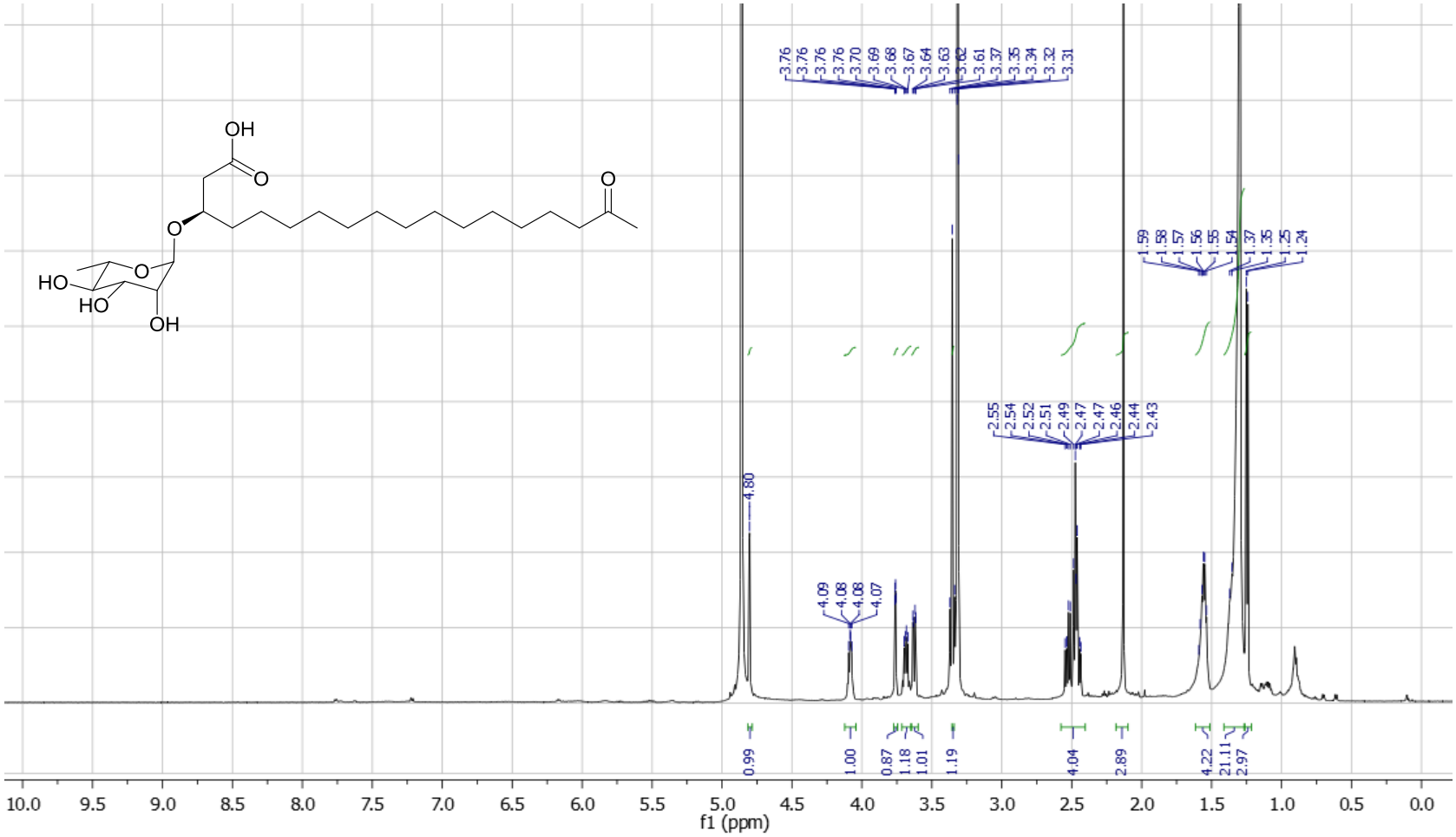

Figure S12. ^{1}H NMR spectrum of dokdolipid B (**2**).

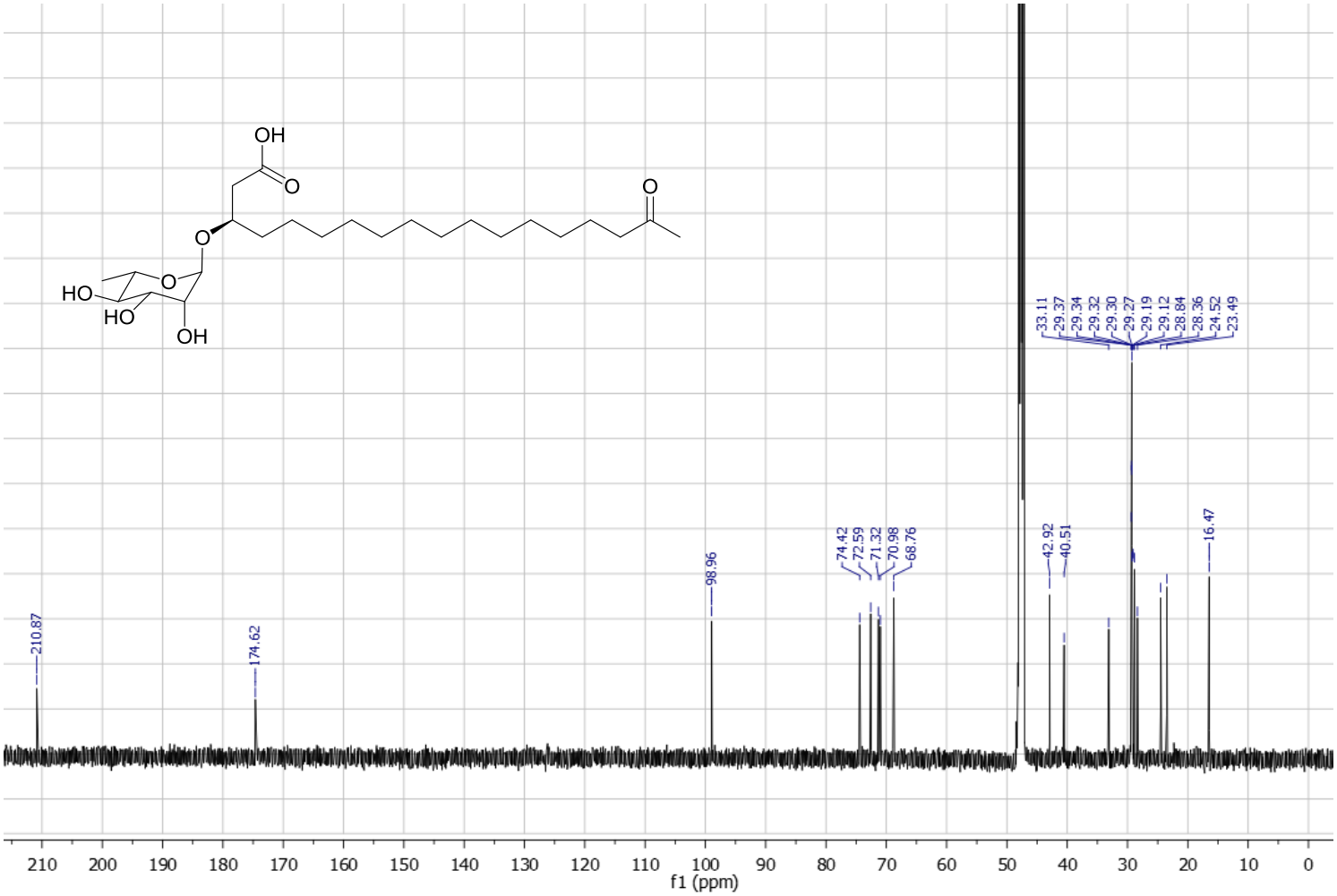

Figure S13. ^{13}C NMR spectrum of dokdolipid B (**2**).

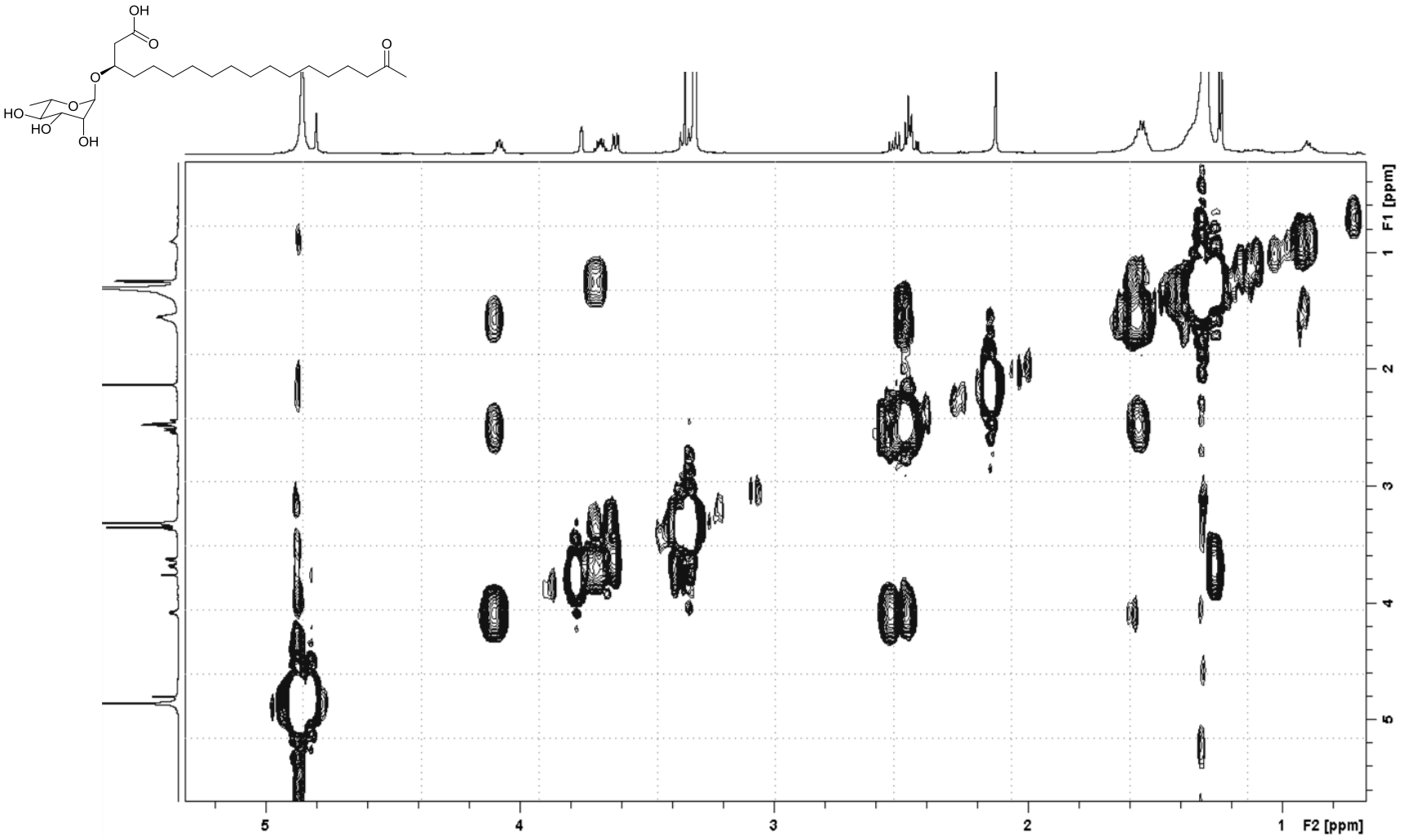

Figure S14. ^{1}H-^{1}H COSY spectrum of dokdolipid B (**2**).

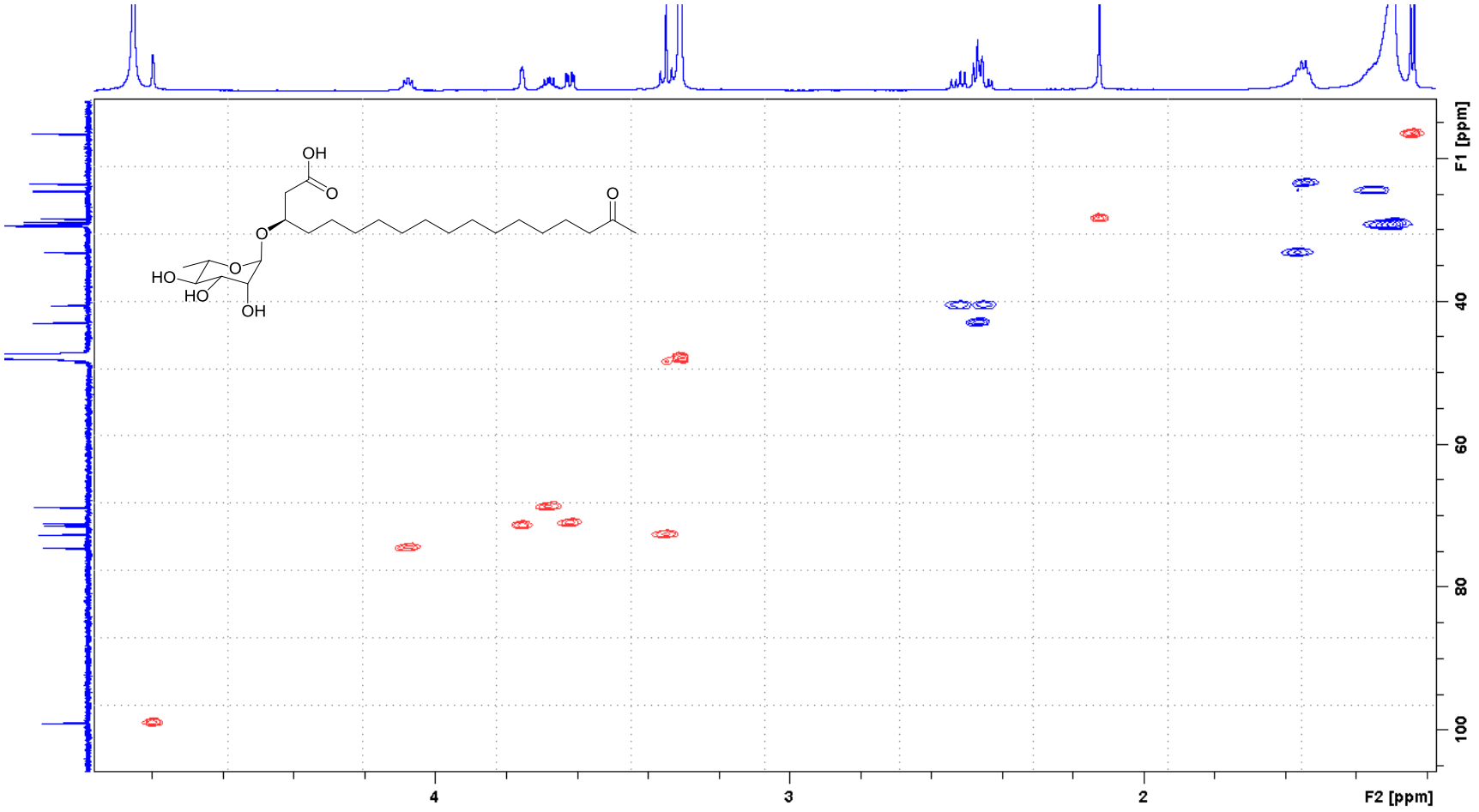

Figure S15. HSQC spectrum of dokdolipid B (**2**).

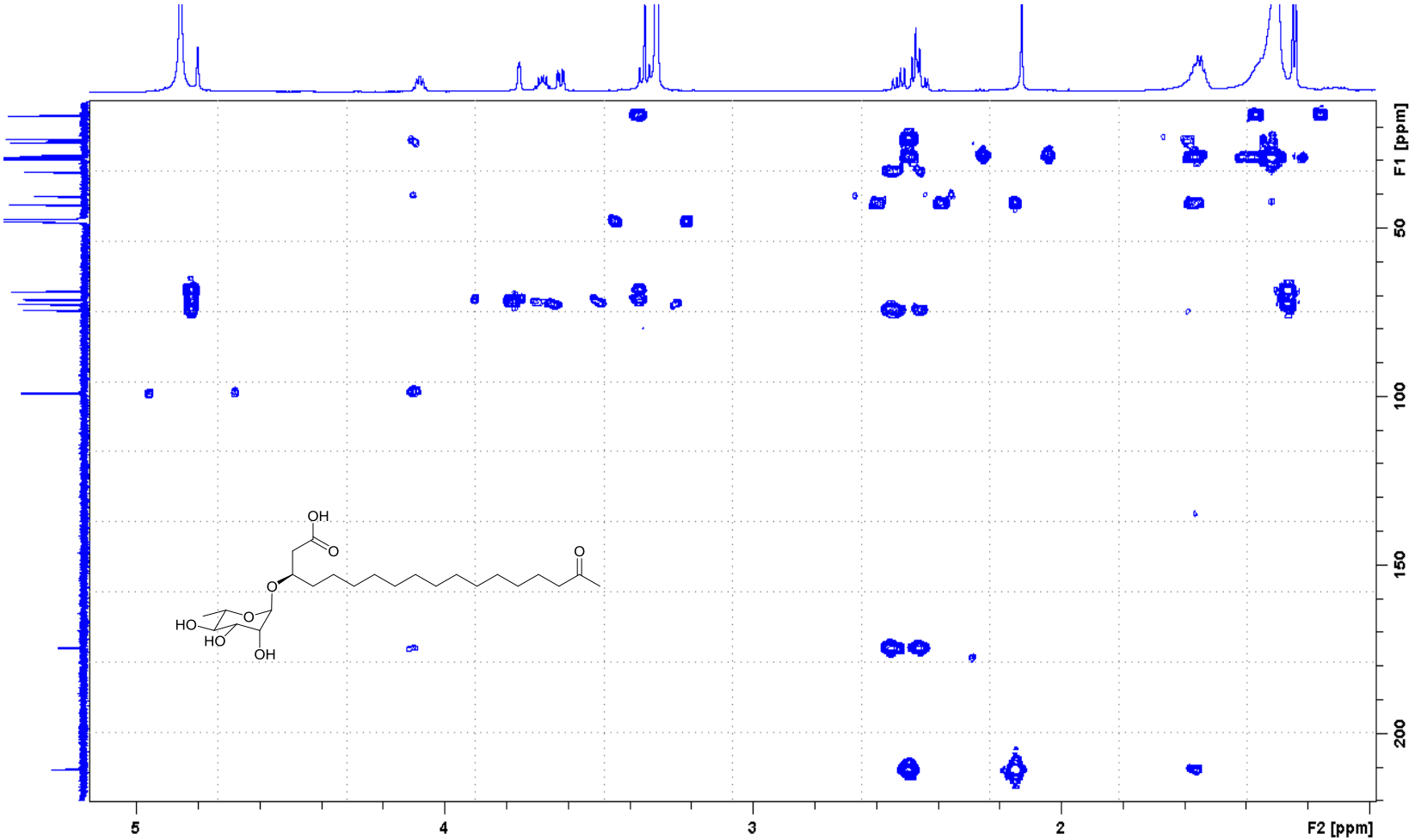

Figure S16. HMBC spectrum of dokdolipid B (**2**).

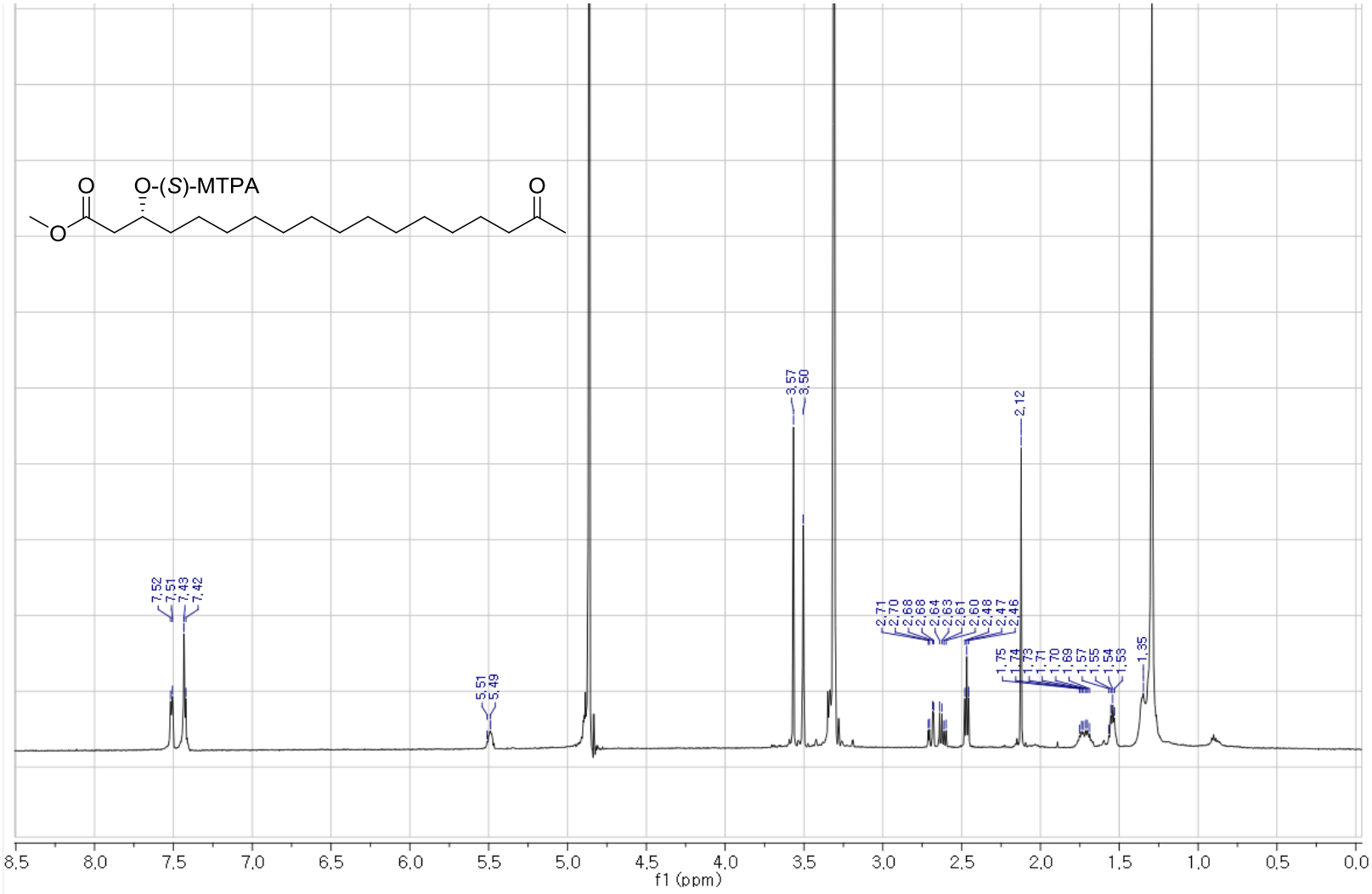

Figure S17. ^{1}H NMR spectrum of (*S*)-MTPA (**2a**) ester.

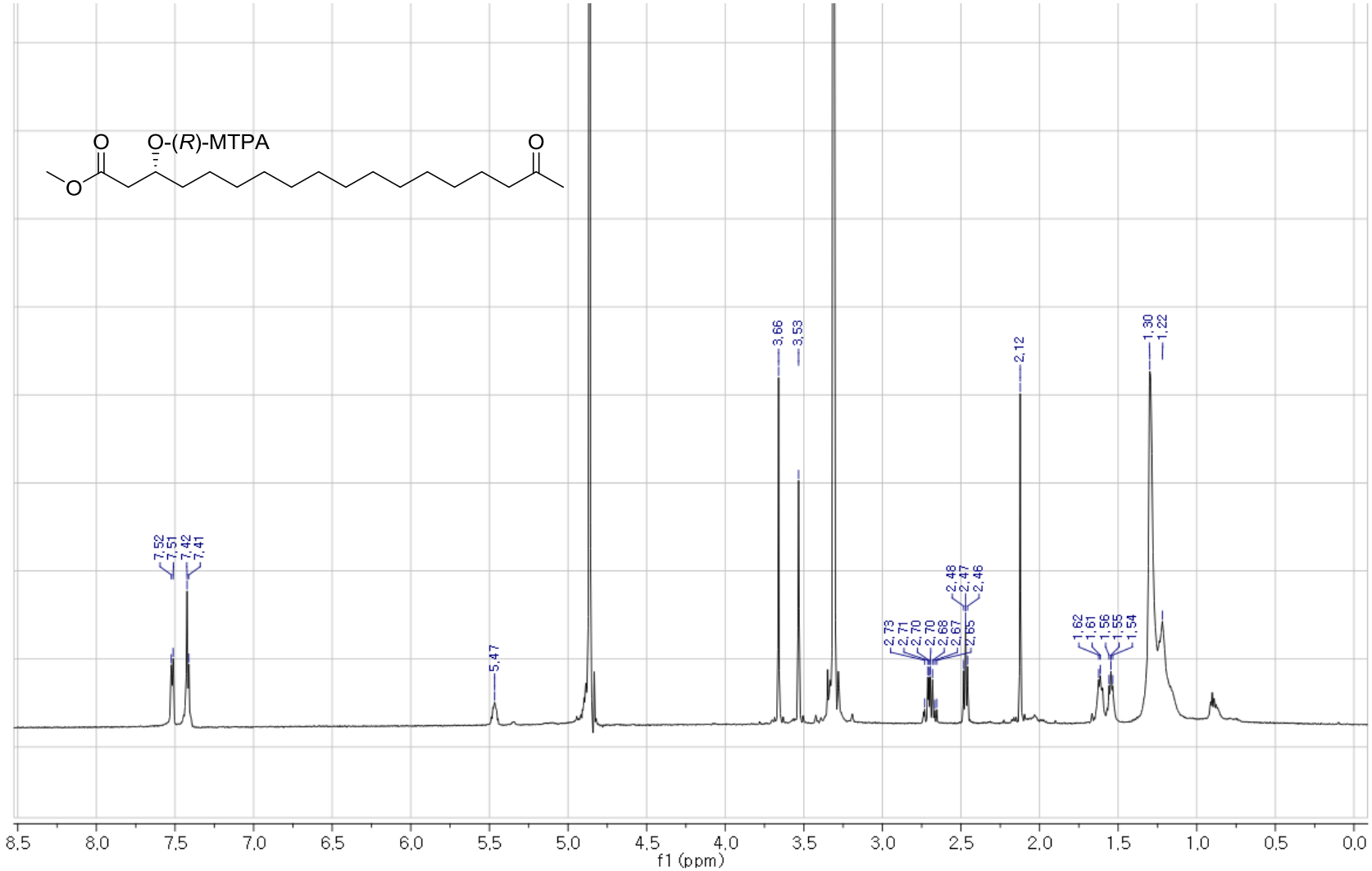

Figure S18. ^{1}H NMR spectrum of (*R*)-MTPA (**2b**) ester.

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Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
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Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-40 H: 1-60 O: 1-20 Na: 1-1

Minimum:				-1.5				
Maximum:		100.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
631.3669	631.3669	0.0	0.0	2.5	694.0	n/a	n/a	C30 H56 O12 Na

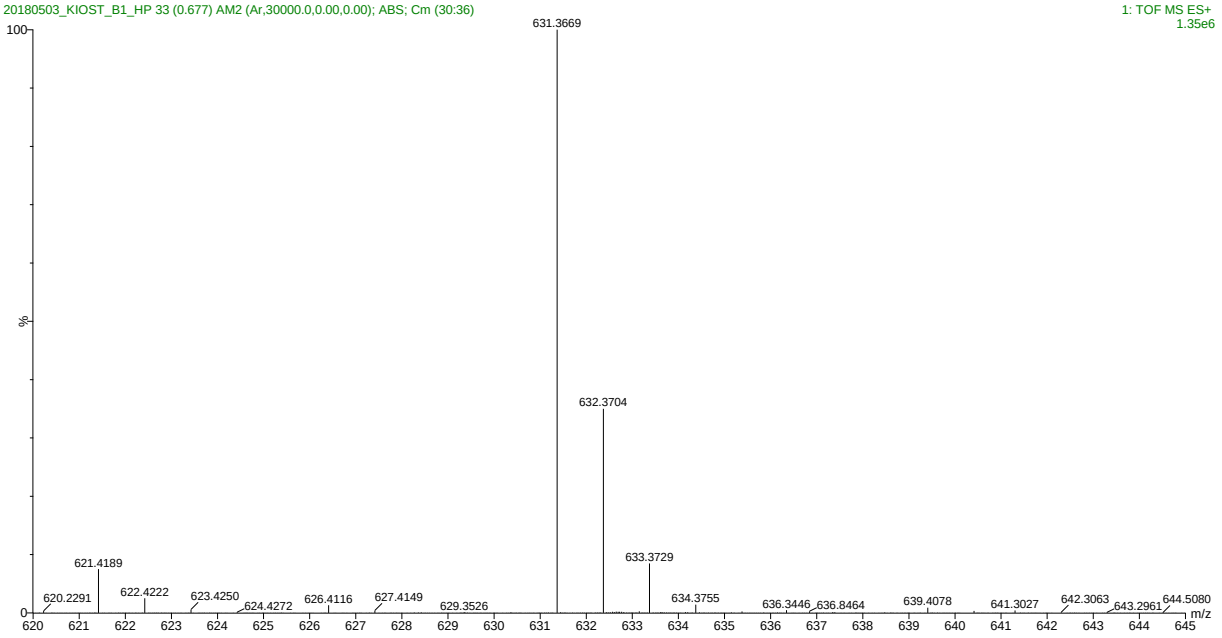

Figure S19. HRESIMS data of dokdolipid C (**3**).

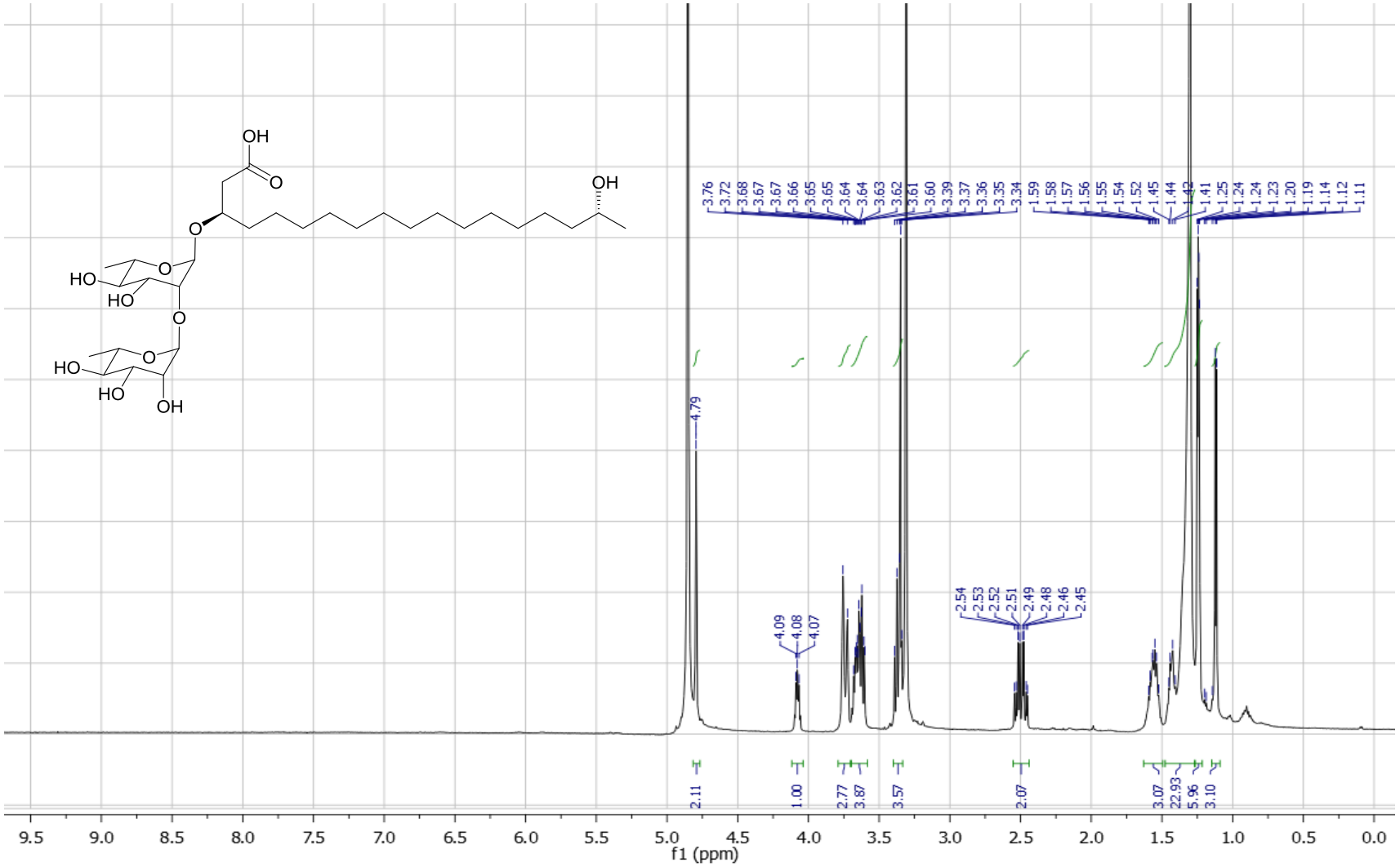

Figure S20. ^{1}H NMR spectrum of dokdolipid C (**3**).

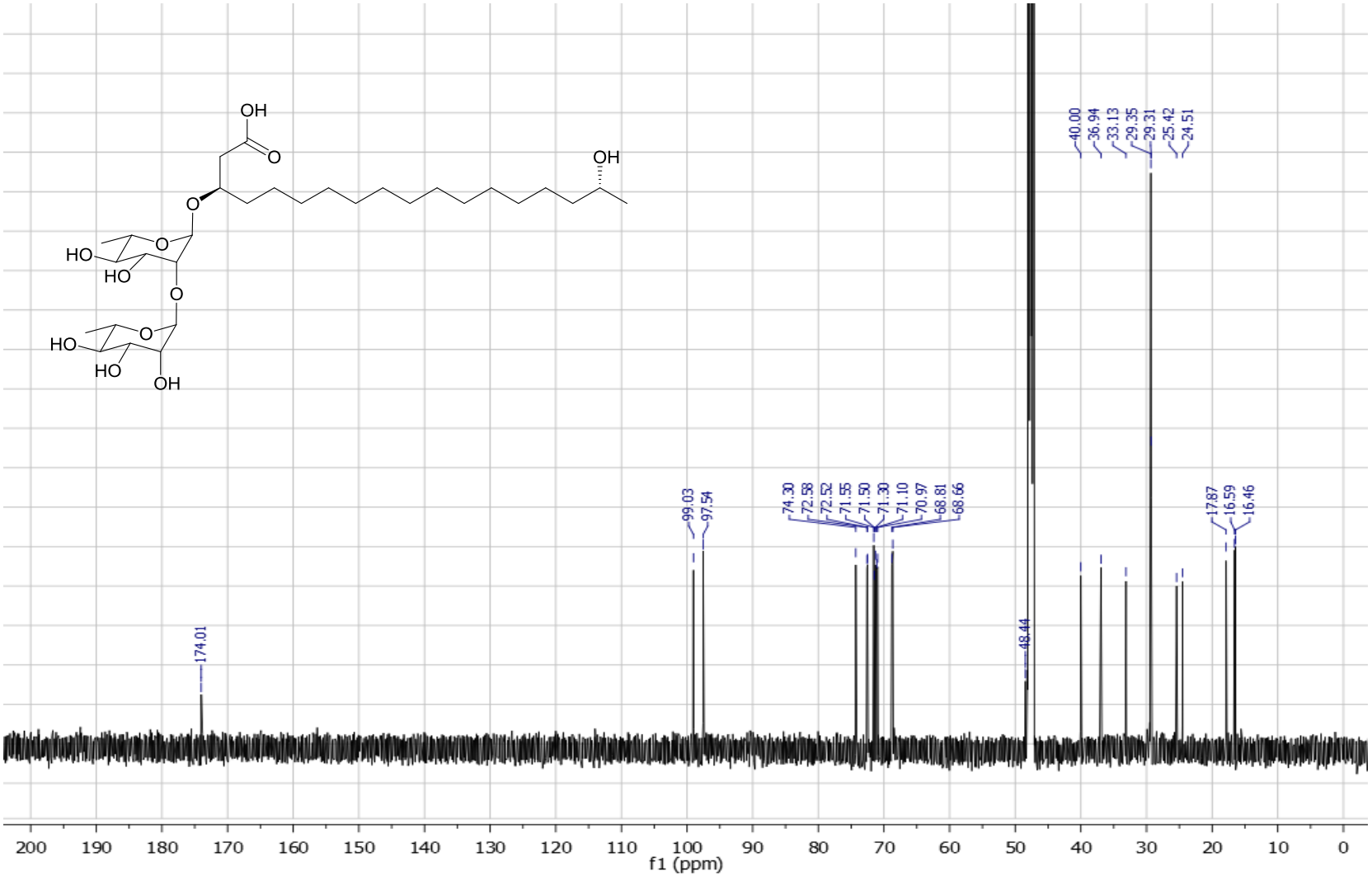

Figure S21. ^{13}C NMR spectrum of dokdolipid C (**3**).

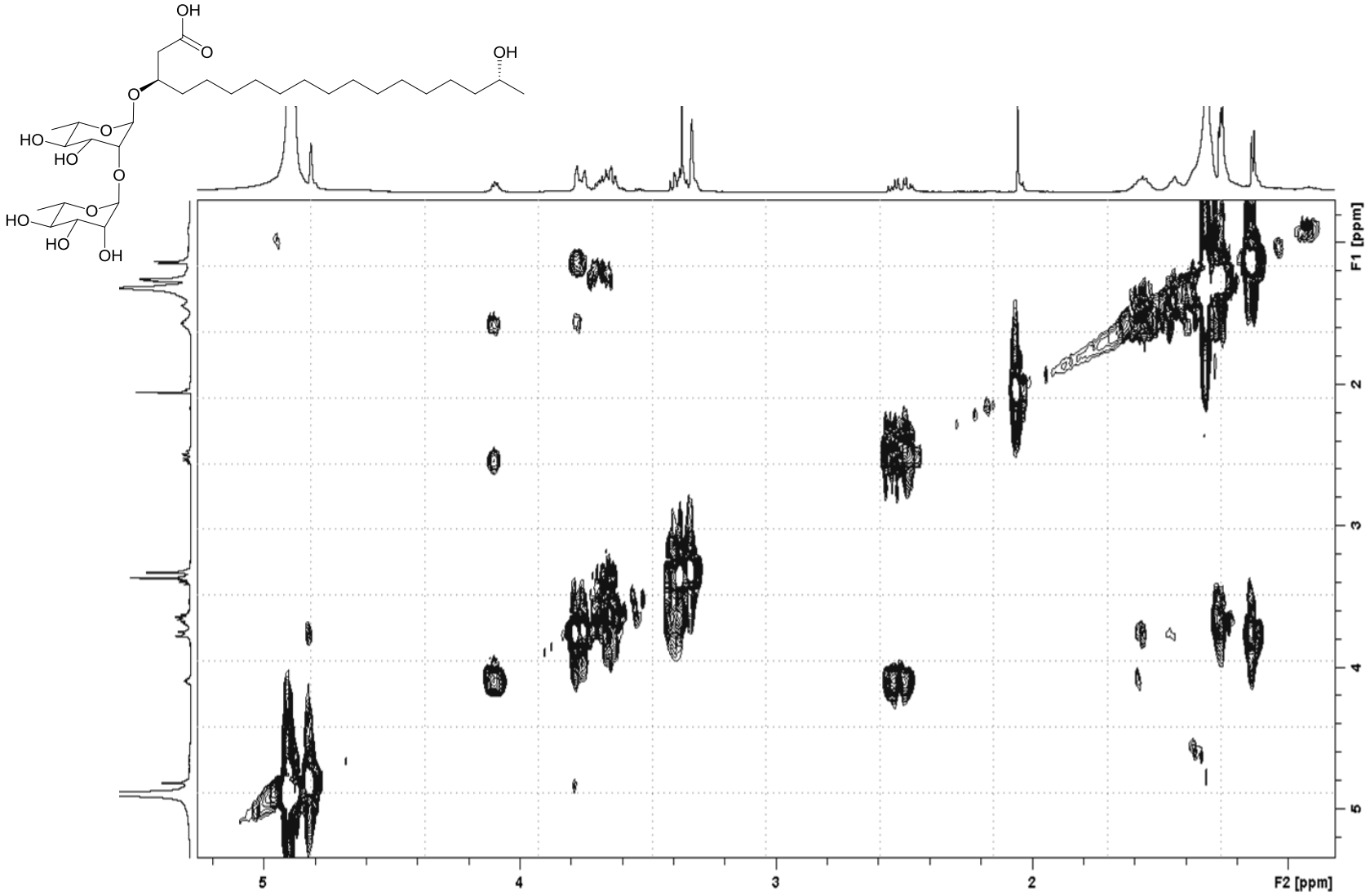

Figure S22. ^{1}H-^{1}H COSY spectrum of dokdolipid C (**3**).

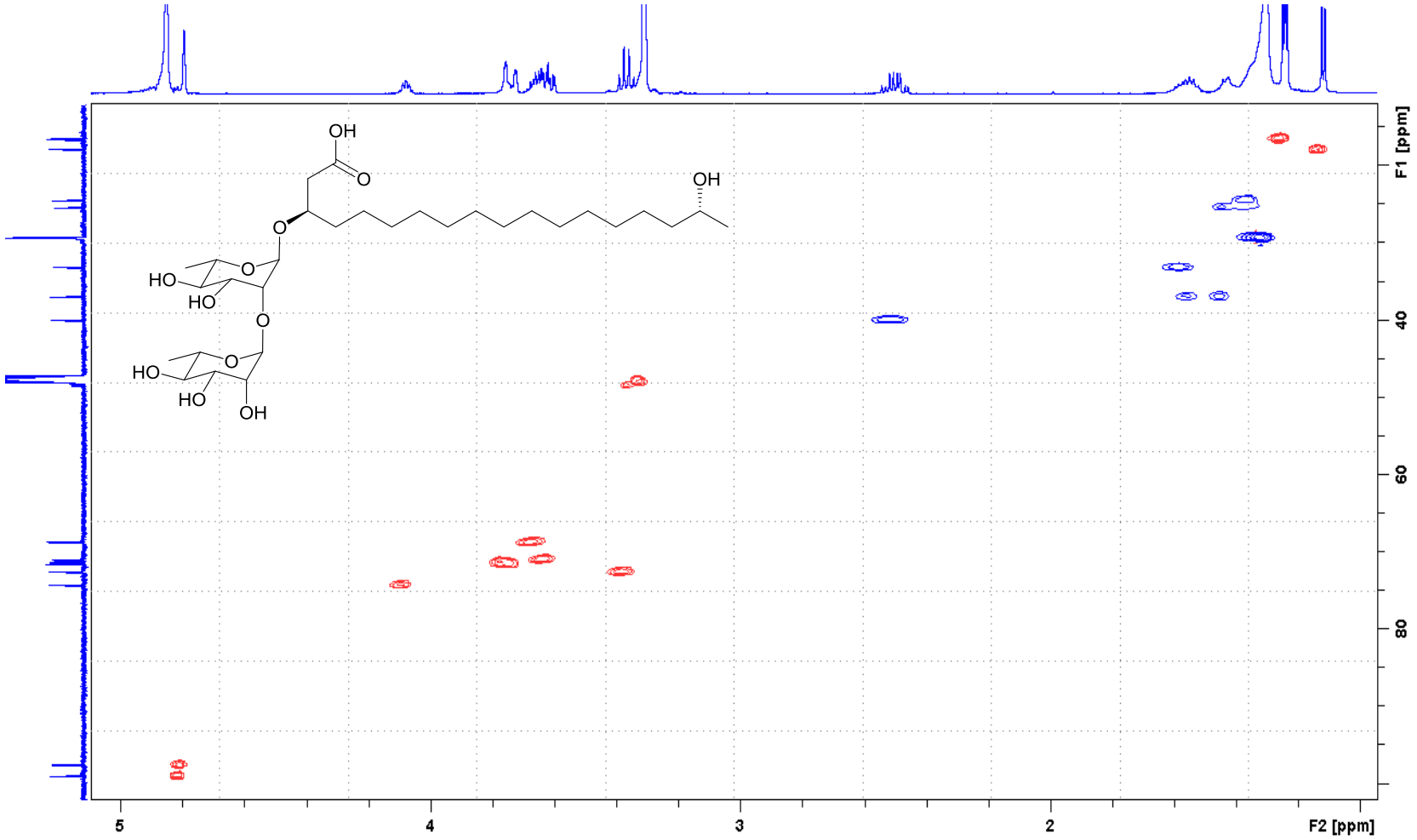

Figure S23. HSQC spectrum of dokdolipid C (**3**).

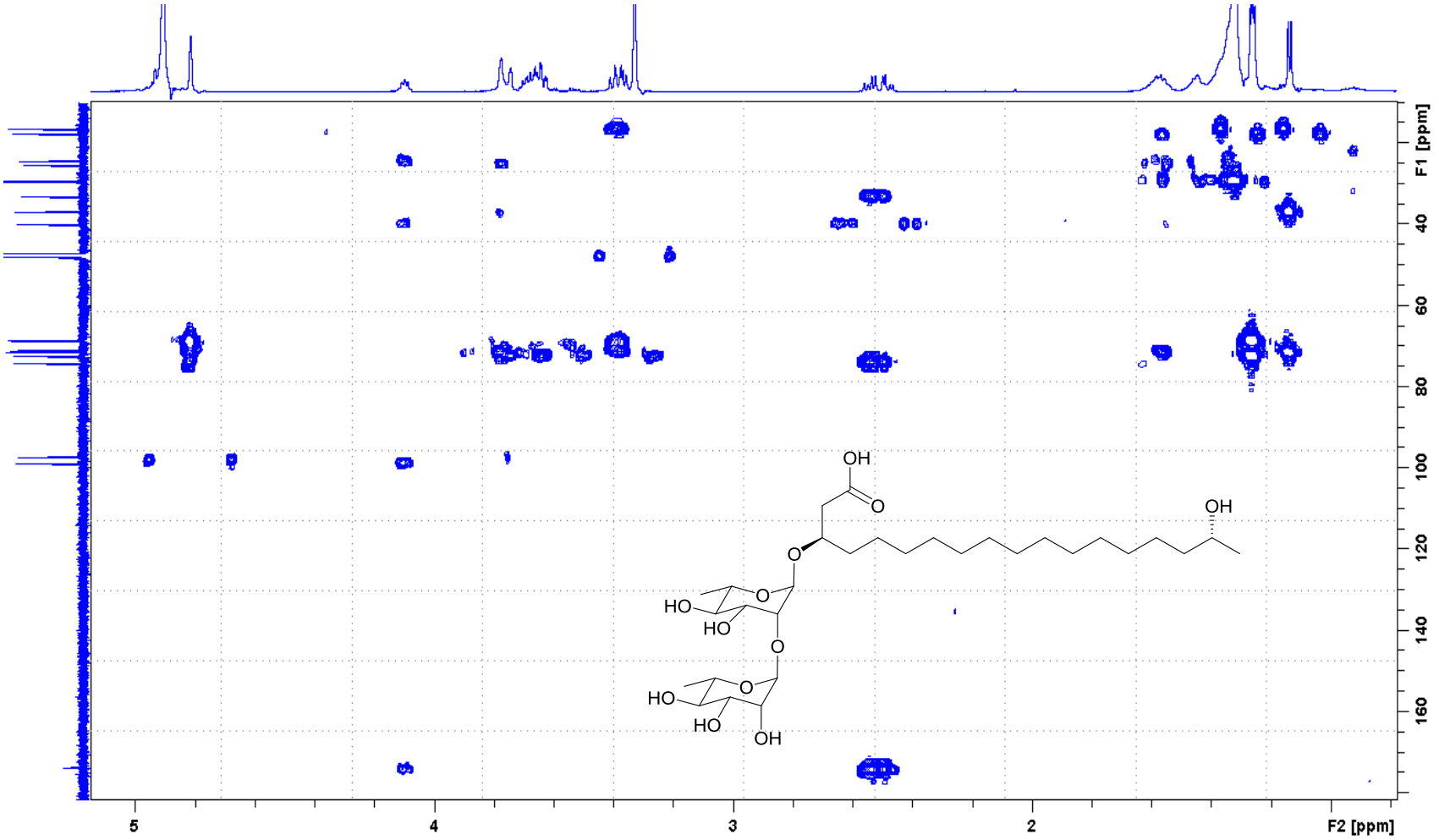

Figure S24. HMBC spectrum of dokdolipid C (**3**).

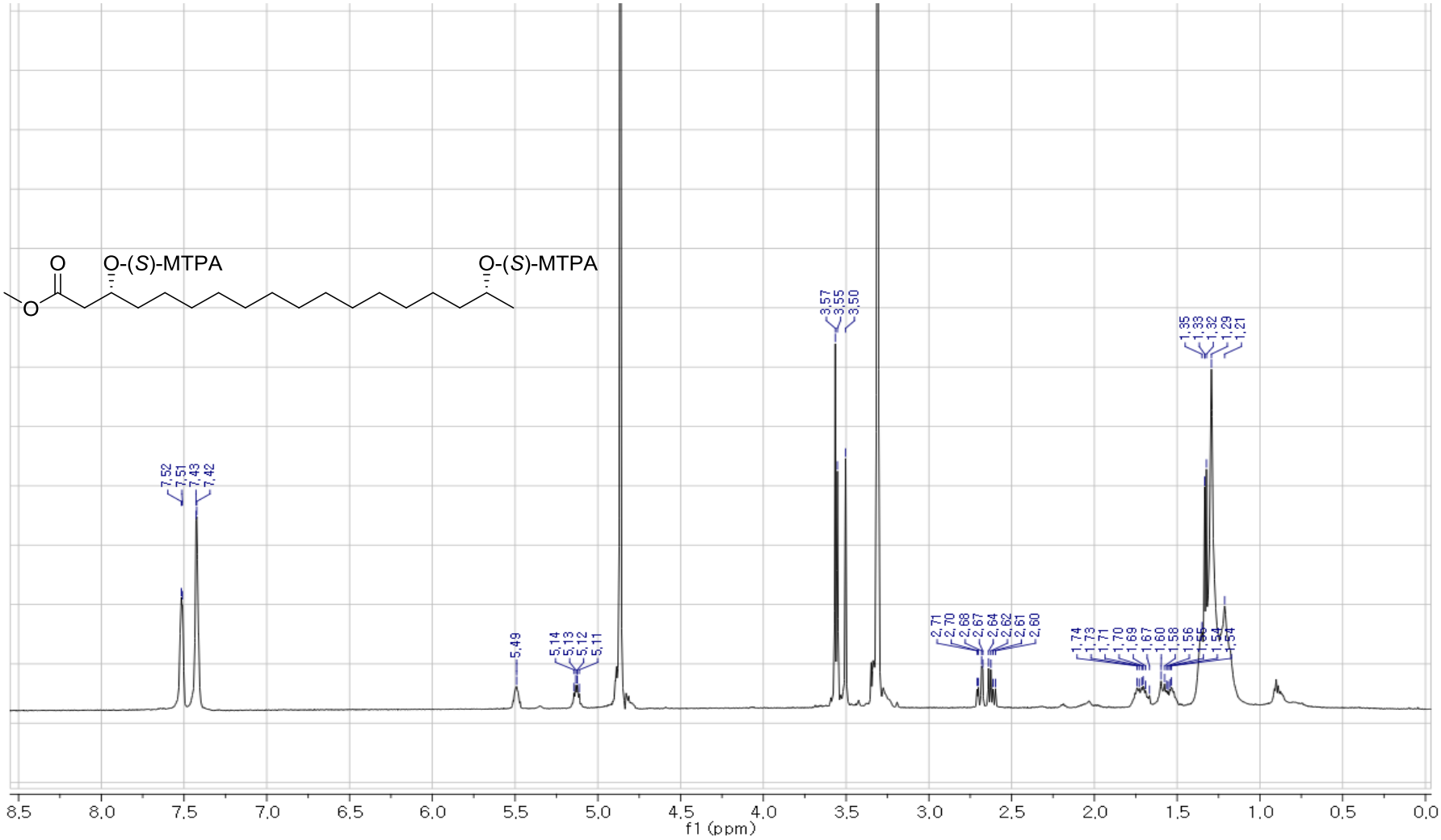

Figure S25. ^{1}H NMR spectrum of (*S*)-MTPA (**3a**) ester.

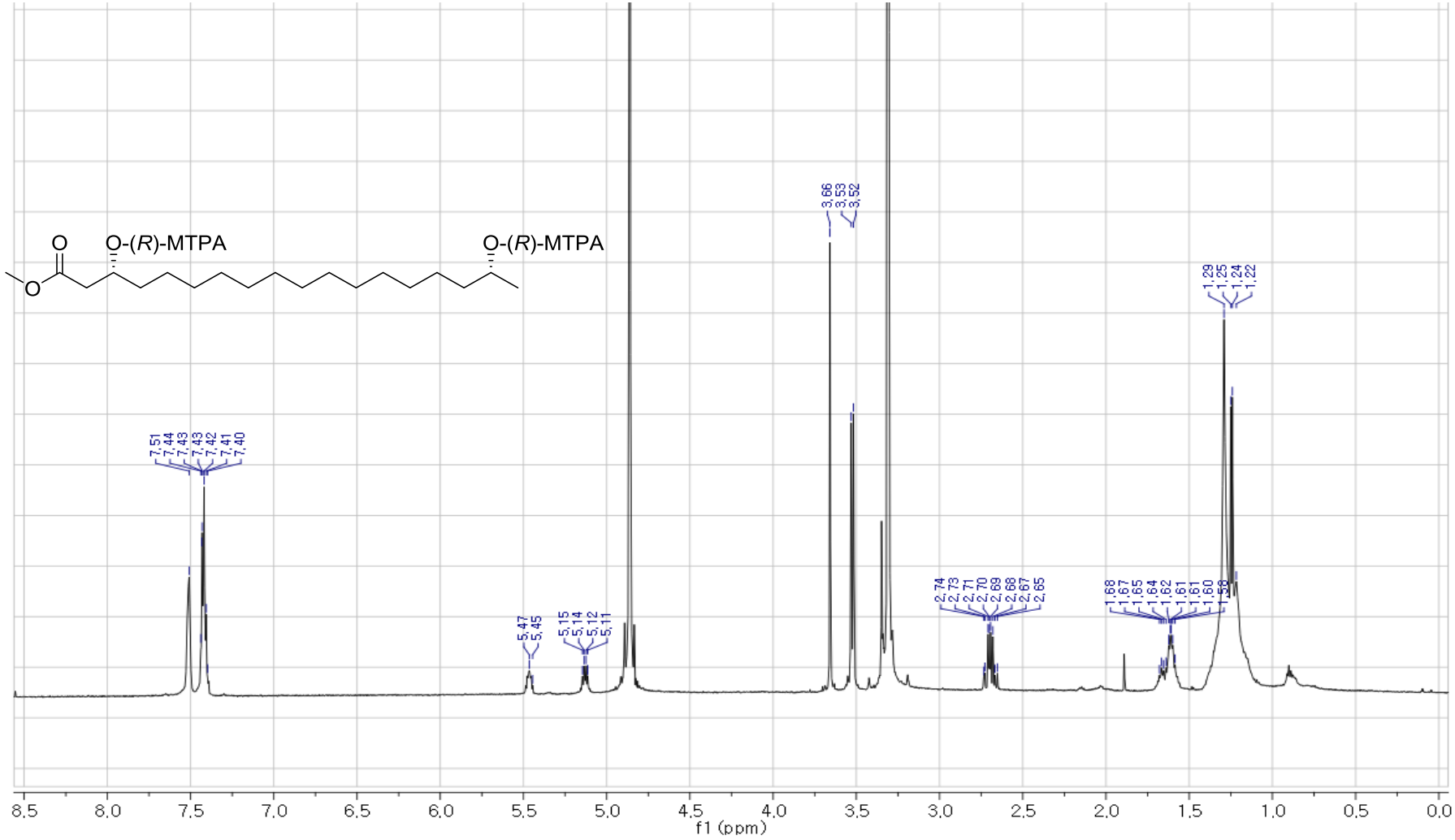

Figure S26. ^{1}H NMR spectrum of (*R*)-MTPA (**3b**) ester.