

Vasorelaxant Effects induced by Red Wine and Pomace extracts of Magliocco dolce *cv.*

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Table S1. ¹H NMR resonance assignment of LDC samples.

Compound	Assignment ^a	¹ H (ppm)	Multiplicity ^b	Sample
Amino acids				
Valine	α -CH	3,62	m	2,4,6
	β -CH	2,29	m	
	γ -CH ₃	1,05	d	
	γ' -CH ₃	1,00	d	
Isoleucine	α -CH	3,69	m	2,4,6
	β -CH	1,99	m	
	γ -CH	1,25	m	
	γ' -CH	1,49	m	
	δ -CH ₃	1,01	d	
	δ' -CH ₃	0,95	t	
Alanine	α -CH	3,77	q	1,2,3,4,5,6
	β -CH ₃	1,49	d	
GABA	α -CH ₂	2,35	t	1,2,3,4
	β -CH ₂	1,91	m	
	γ -CH ₂	3,02	t	
Glutamate	α -CH	α -CH	3,74	2
	β -CH ₂	β -CH ₂	2,08	
	γ -CH ₂	γ -CH ₂	2,36	
Glutamine	α -CH	α -CH	3,76	2
	β -CH ₂	β -CH ₂	2,11	
	γ -CH ₂	γ -CH ₂	2,45	
Tyrosine	C2,6H-ring	6,88	m	4
	C3,5H-ring	7,18	m	
Phenylalanine	C2,6H-ring	7,33	m	2,4,6
	CH-4 ring	7,39	m	
	C3,5H-ring	7,42	m	
Tryptophan	CH-2 ring	7,31	s	2,4,6
	CH-4 ring	7,27	d	
	CH-5 ring	7,19	m	
	CH-6 ring	7,72	m	
	CH-7 ring	7,53	d	
Organic Acids				

Lactic acid	α -CH β -CH	4,12 1,37	q d	2,3,4
Quinic Acid	CH ₂ -1 CH-2 CH-3 CH-4 CH ₂ -5	1,89, 2,09 4,02 3,55 4,15 2,00, 2,06	dd m m m dd	1,2,3,4
Succinic acid	α,β -CH ₂	2,41	s	2,3,4,6
Malic acid	α -CH β -CH ₂ β' -CH ₂	4,28 2,34 2,65	dd dd dd	1,2,3,4
Fumaric acid	α,β -CH=CH	6,51	s	1,2
p-Coumaric acid	α -CH β -CH CH-2,6 CH-3,5	6,36 7,49 6,80 7,51	d d m m	2
Gallic acid	CH-2,6	7,05	s	1,2,3,4,5,6
Caffeic acid	α -CH β -CH CH-2 CH-5 CH-6	6,42 7,42 7,22 6,96 7,14	d d d d dd	2
Formic acid	CH	8,46	s	1,2,3,4,5,6
Carbohydrates				
α -Glucose	CH-1 CH-2 CH-3 CH-4 CH-5 CH ₂ -6	5,23 3,55 3,72 3,42 3,84 3,73 – 3,90	d m m m m m	1,2,3,4,5,6
β -Glucose	CH-1 CH-2 CH-3 CH-4 CH-5 CH ₂ -6	4,65 3,24 3,50 3,42 3,48 3,74 – 3,91	d dd m m m m	1,2,3,4,5,6

Sucrose	GLC CH-1	5,42	d	1,6
	CH-2	3,59	m	
	CH-3	3,79	m	
	CH-4	3,48	m	
	CH-5	3,85	m	
	CH ₂ -6	3,82	m	
	FRU CH ₂ -1'	3,69	m	
	CH-3'	4,22	d	
	CH-4'	4,06	m	
	CH-5'	3,90	m	
CH ₂ -6	3,82	m		
Fructose	CH ₂ -1	3,69	m	2,3,5,6
	CH-3	4,20	d	
	CH-4	4,06	m	
	CH-5	3,90	m	
CH ₂ -6	3,82	m		
Miscellaneous Compounds				
2,3-butanediol	CH₃-1	1,16	d	2,3,6
	CH-2	3,65	m	
	CH-3	3,74	m	
	CH ₃ -4	1,17	d	
Catechin	CH-6	6,12	d	2,3,5,6
	CH-8	6,14	d	
	CH-2'	6,95	d	
	CH-5'	6,75	d	
	CH-6'	6,68	dd	
	CH-2''	4,56	d	
	CH-3''	3,97	m	
	CH ₂ -4''	2,49, 2,82	dd	
Quercetin-3-O-Galactoside	CH-6	6,20	d	1,2,3
	CH-8	6,41	d	
	CH-2'	7,69	d	
	CH-5'	6,91	d	
	CH-6'	7,55	dd	
	CH-1''	5,48	d	
	CH-2''	3,80	m	
	CH-3''	3,87	m	
	CH-4''	3,98	m	

	CH-5''	4,08	m	
	CH2-6''	3,73	m	
Nicotinamide riboside	C2H Nam	9,61	s	1,2,3,4,5,6
	C4H Nam	8,89	m	
	C5H Nam	8,31	m	
	C6H Nam	9,34	m	

^a specific resonance signal used for quantization are reported in bold

^b s: singlet; d: doublet; dd: double doublet; t: triplet; q: quartet; m: multiplet

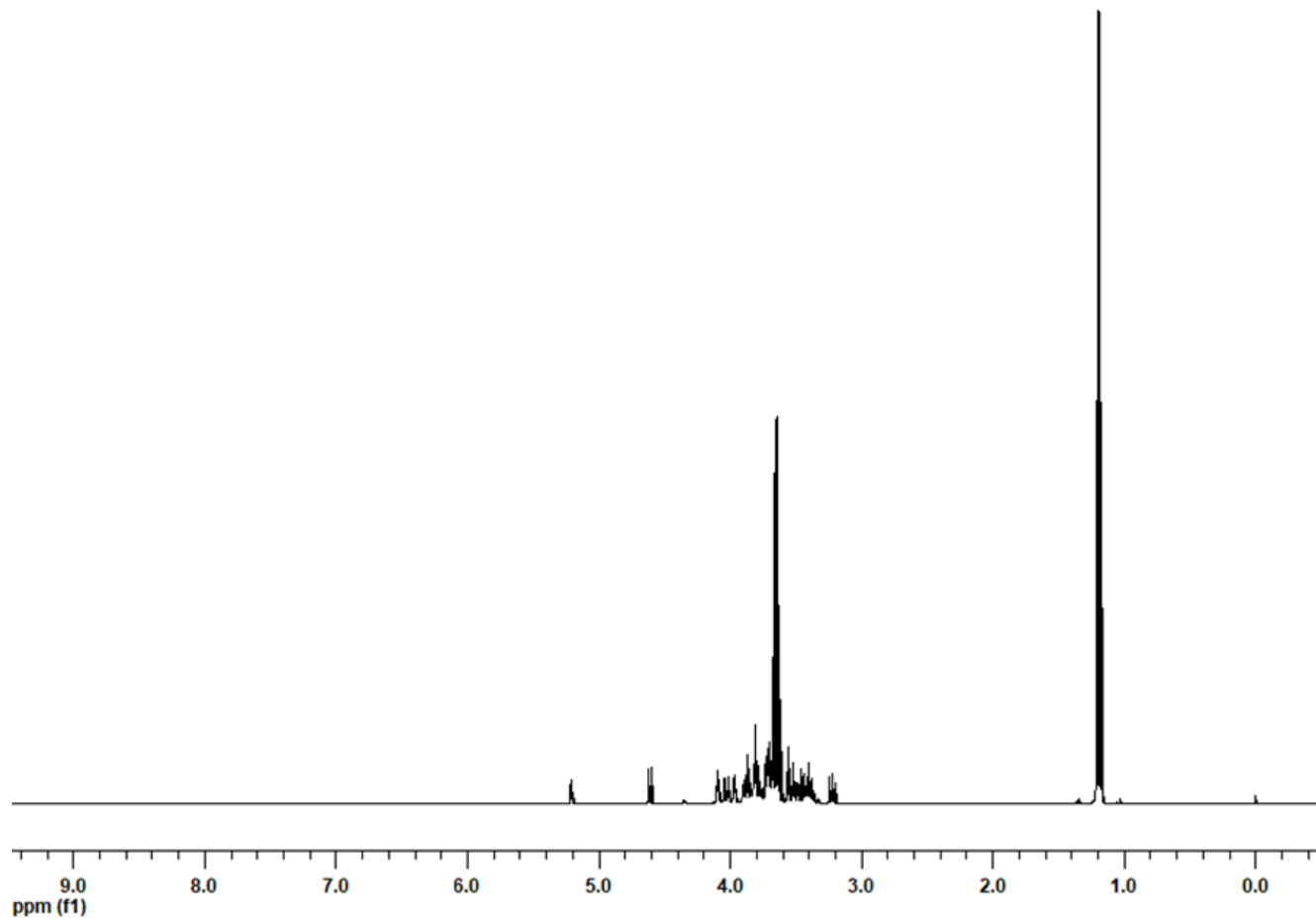


Figure S1: 1D ^1H NMR spectrum of LDC1

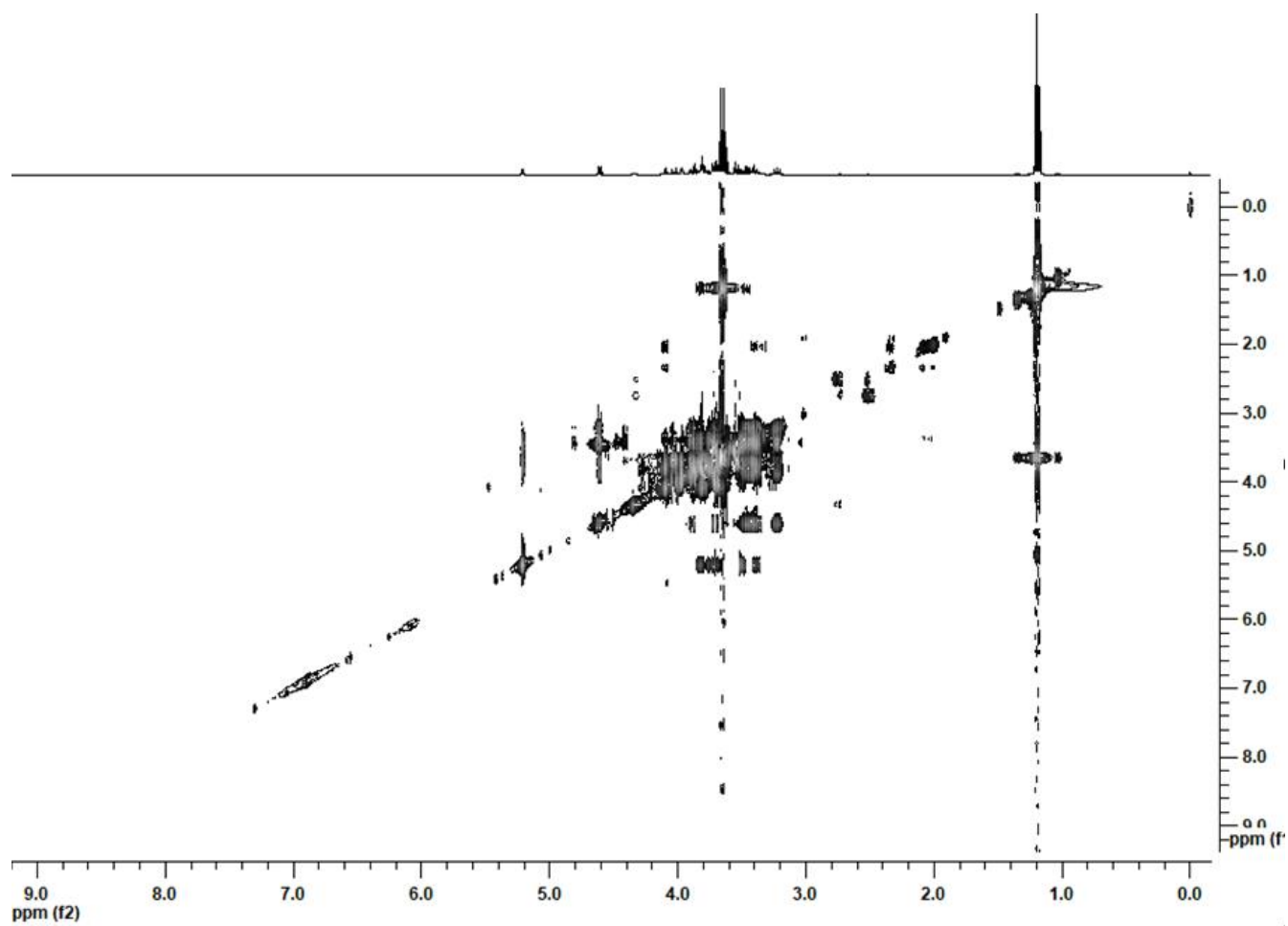


Figure S2: ^1H - ^1H TOCSY NMR spectrum of LDC1

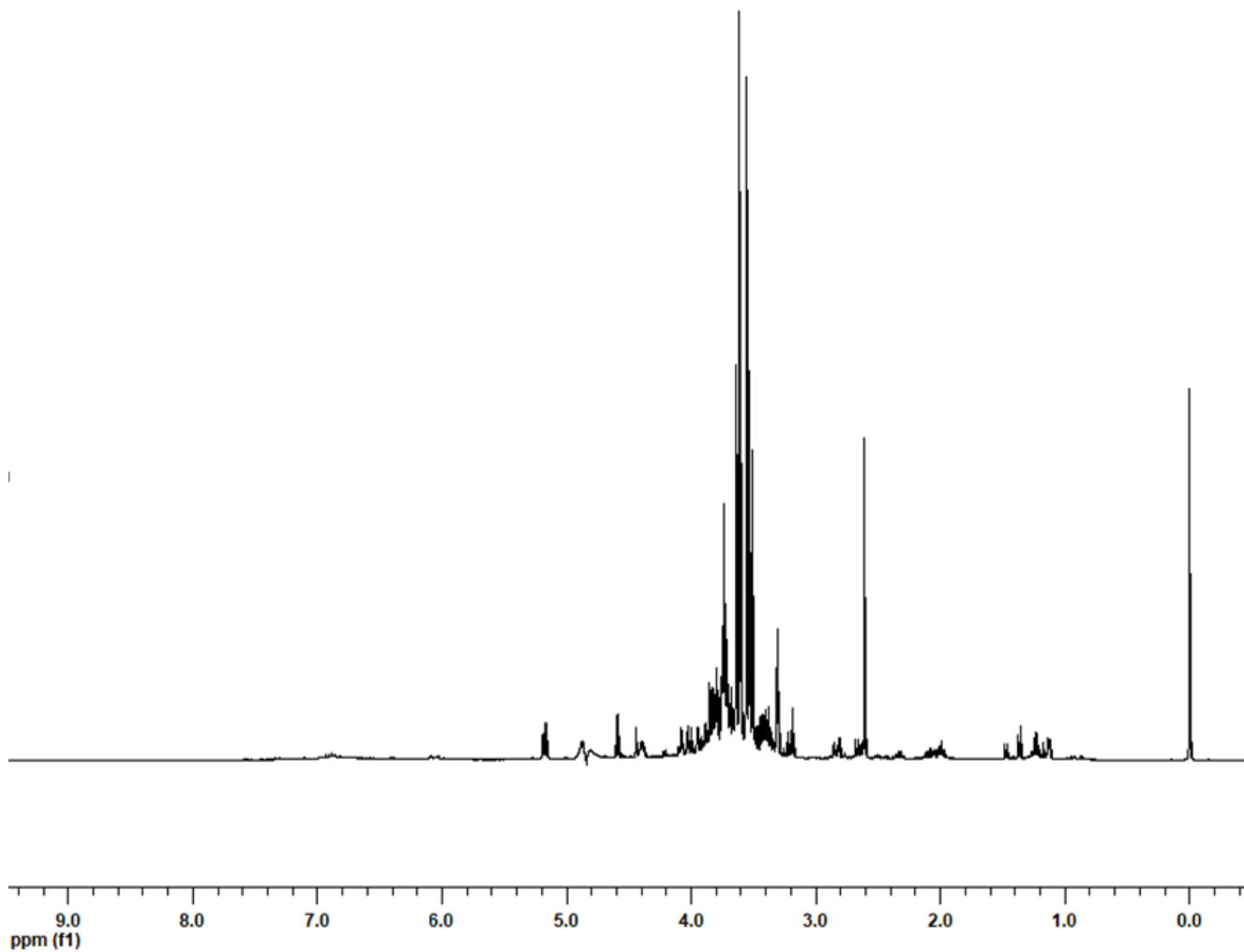


Figure S3: 1D ^1H NMR spectrum of LDC2

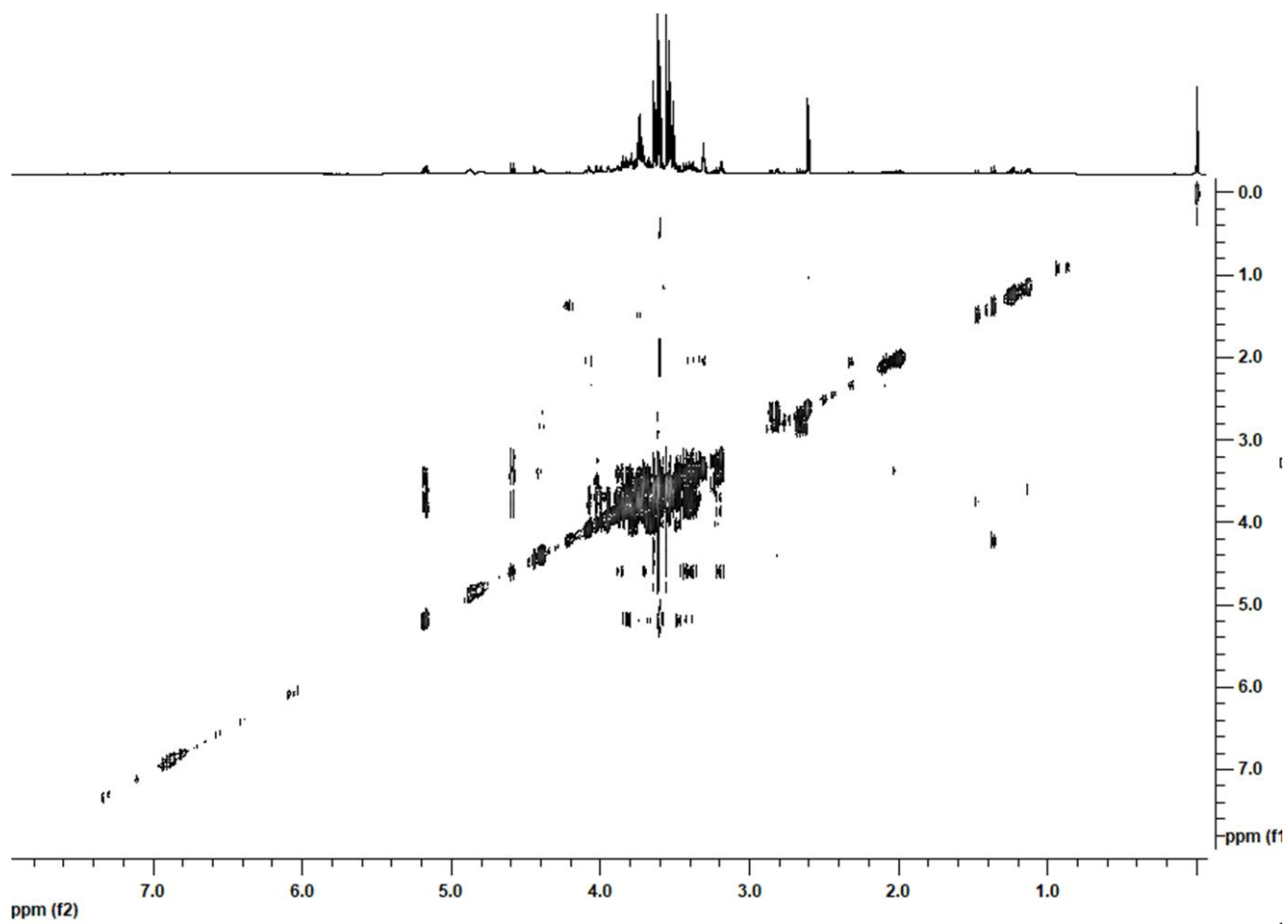


Figure S4: ¹H-¹H TOCSY NMR spectrum of LDC2

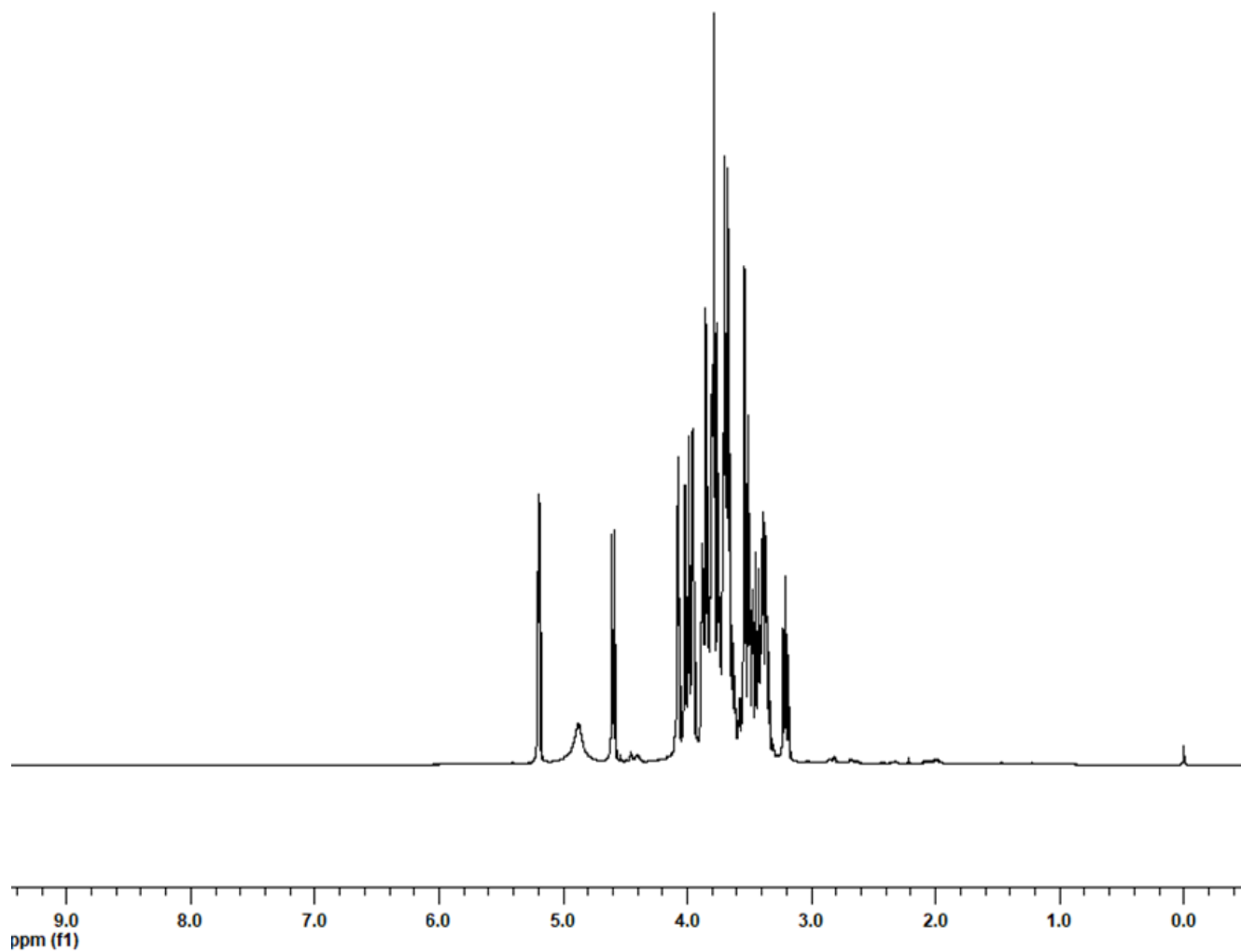


Figure S5: 1D ^1H NMR spectrum of LDC4

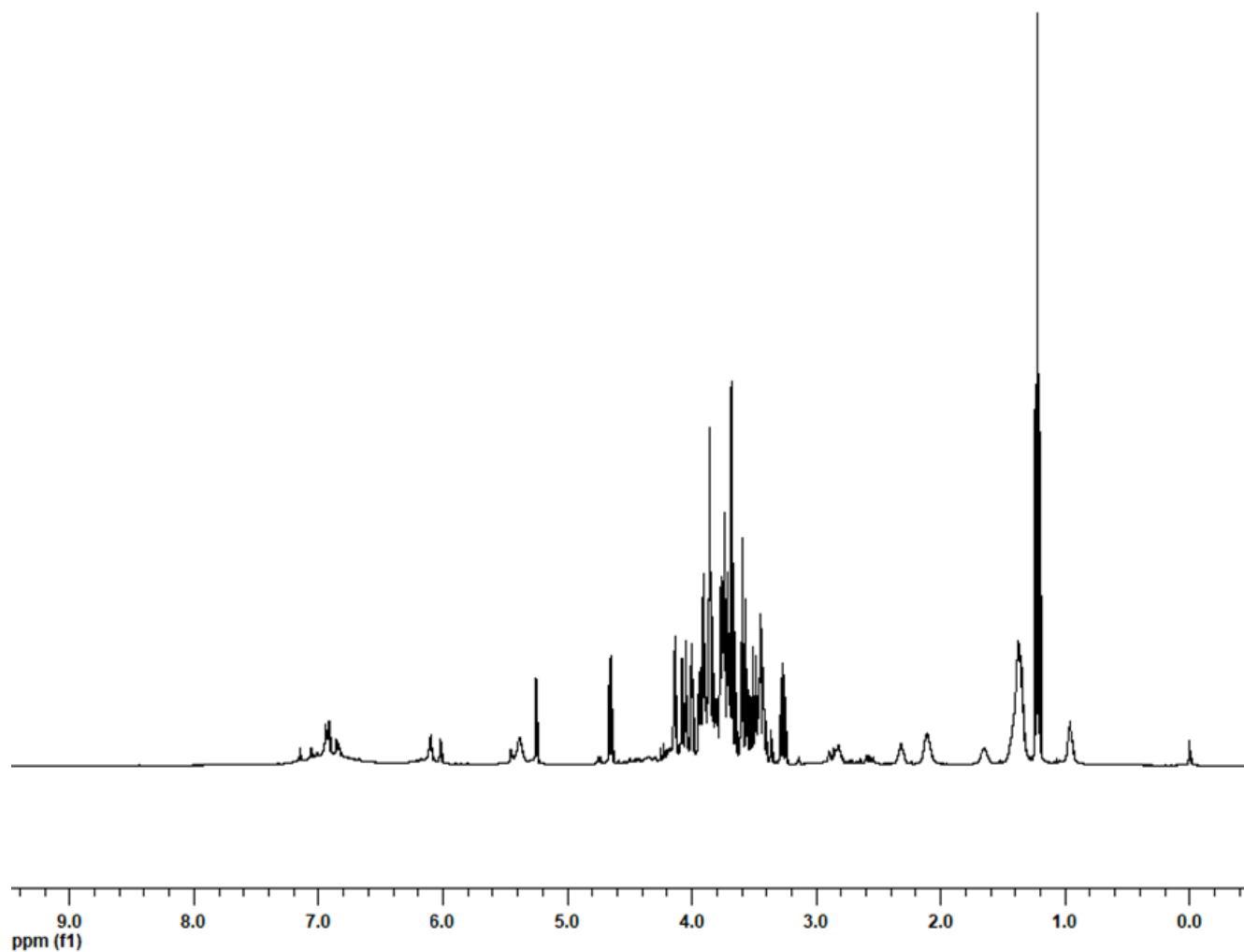


Figure S6: 1D ^1H NMR spectrum of LDC5

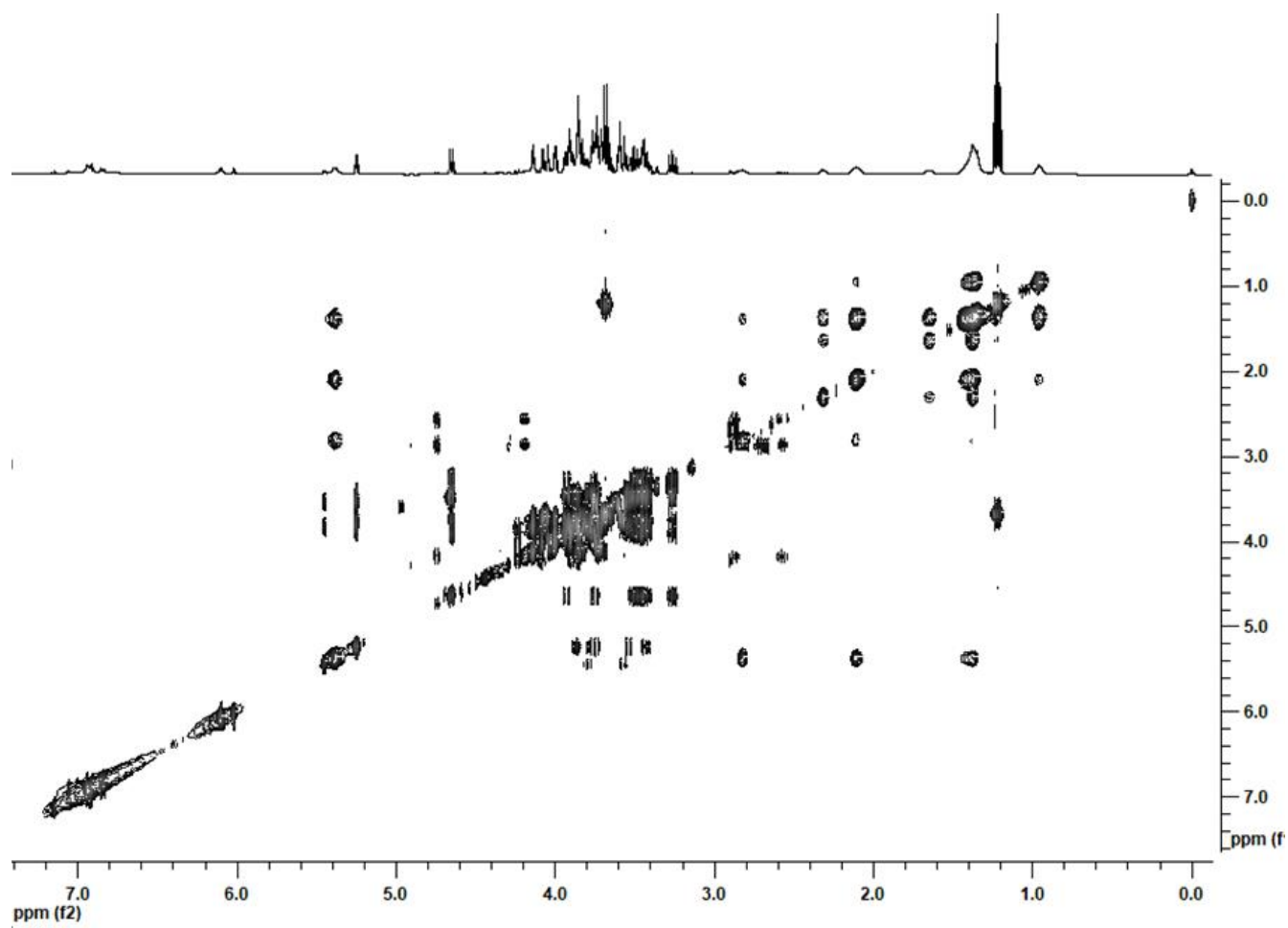


Figure S7: ^1H - ^1H TOCSY NMR spectrum of LDC5

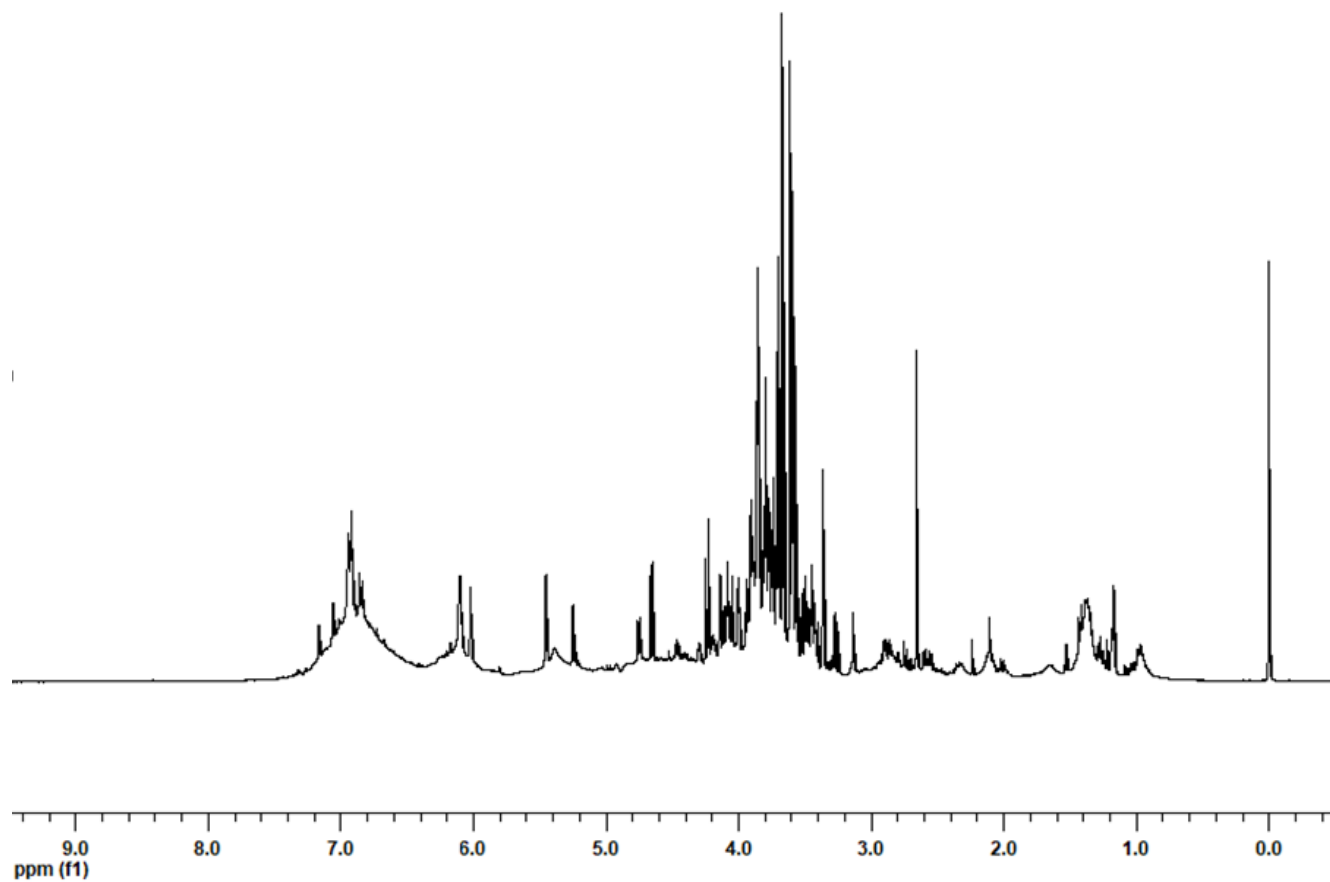


Figure S8: 1D ^1H NMR spectrum of LDC6