Supplementary data

On the Inhibitability of Natural Products Isolated from *Tetradium ruticarpum* towards Tyrosine Phosphatase 1B (PTP1B) and α-glucosidase (3W37): an *in vitro* and *in silico* Study

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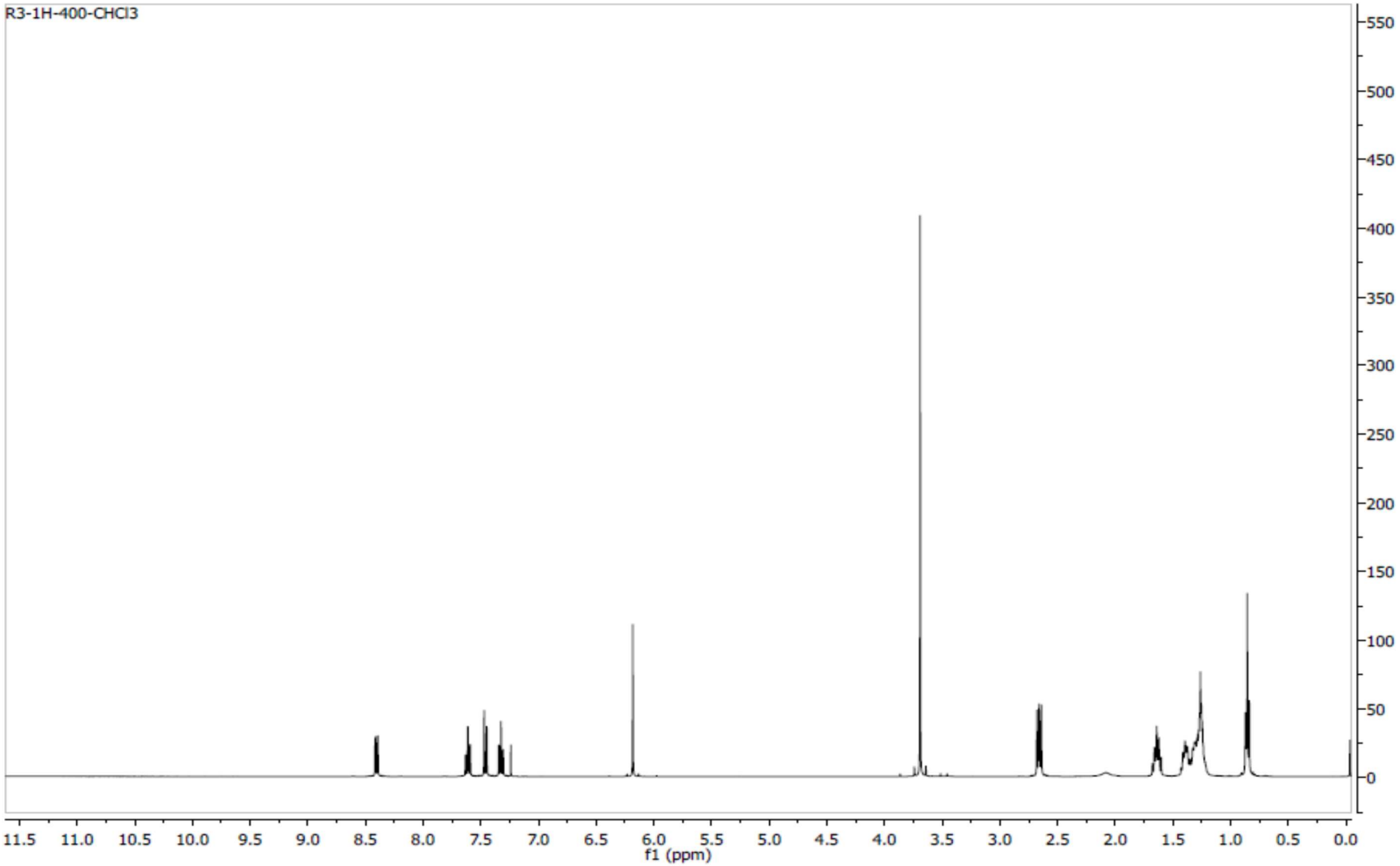

Figure S1. ^{1}H NMR spectrum of compound **1** (400 MHz, $CDCl_3$)

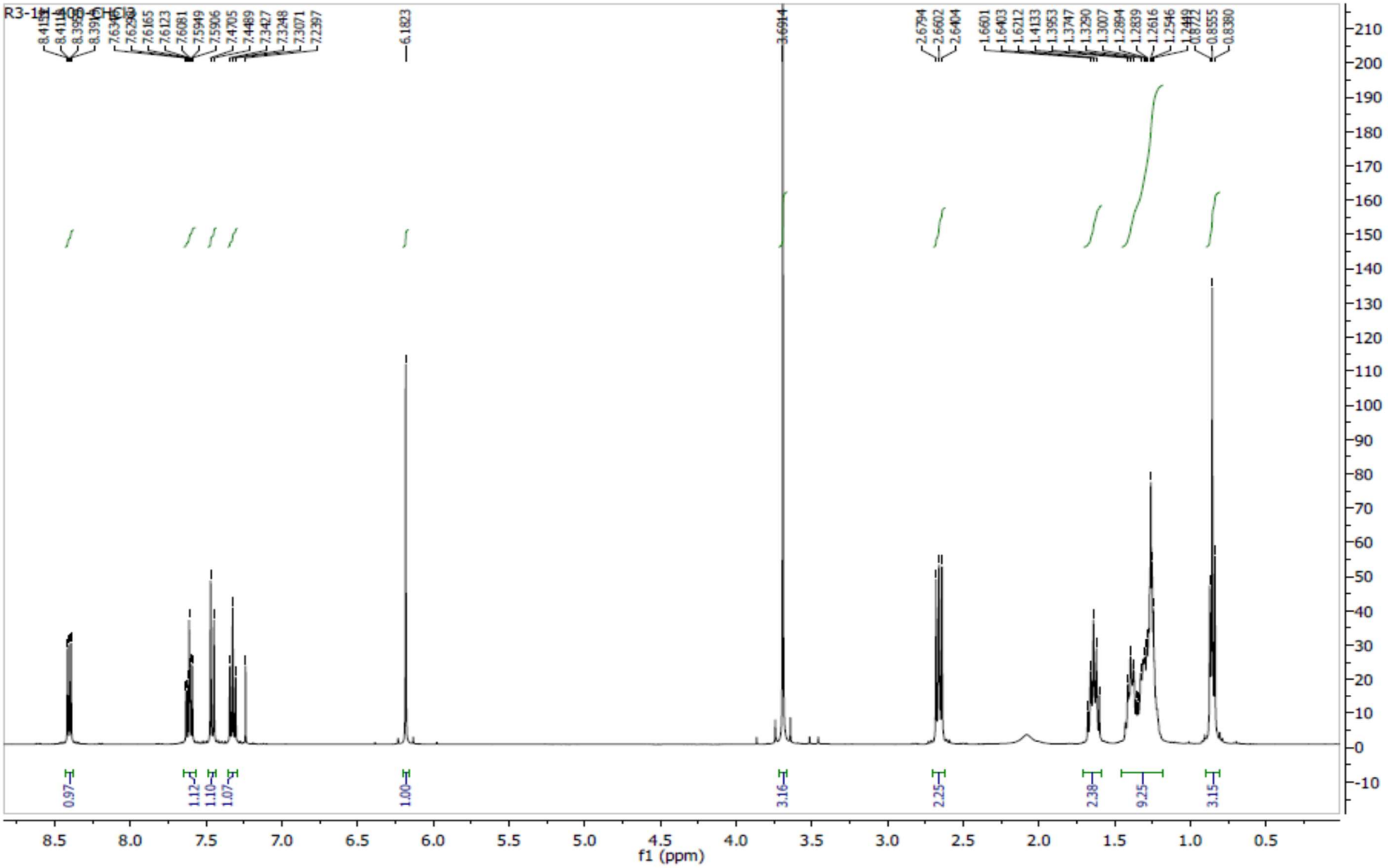

Figure S2. ^{1}H NMR spectrum of compound **1** (400 MHz, $CDCl_3$) (expanded)

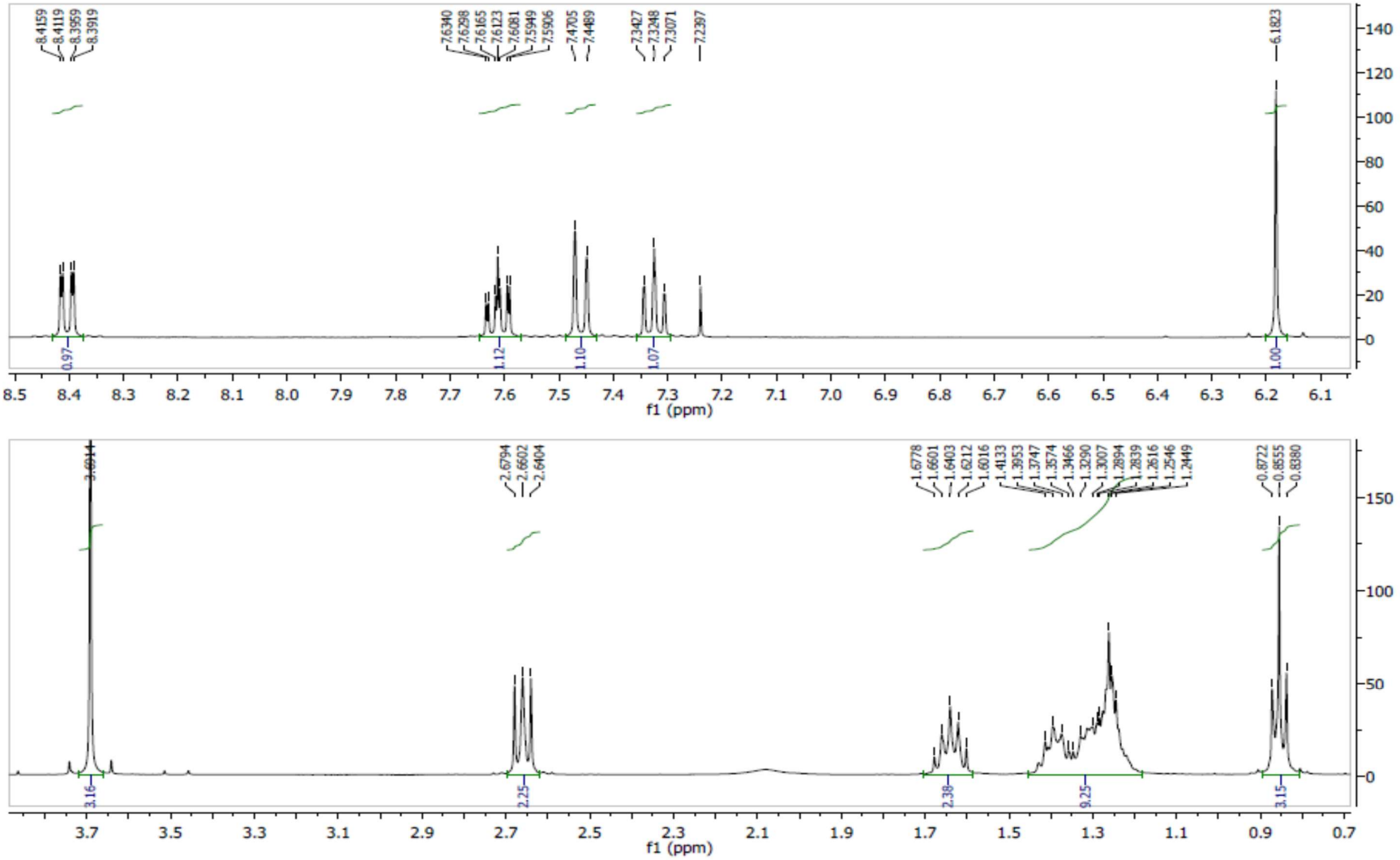

Figure S3. ^{1}H NMR spectrum of compound **1** (500 MHz, $CDCl_3$) (expanded)

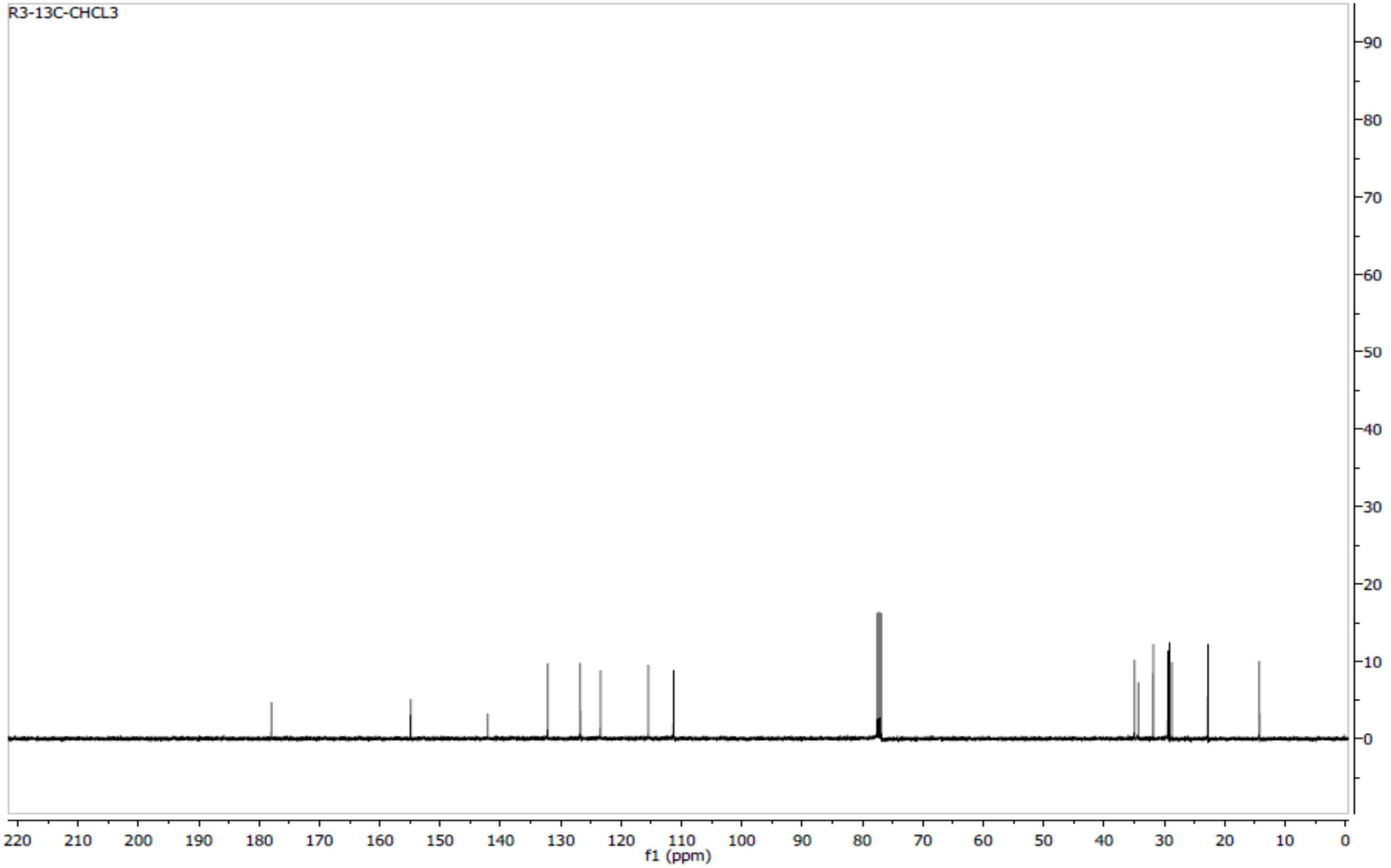

Figure S4. ^{13}C NMR spectrum of compound **1** (100 MHz, $CDCl_3$)

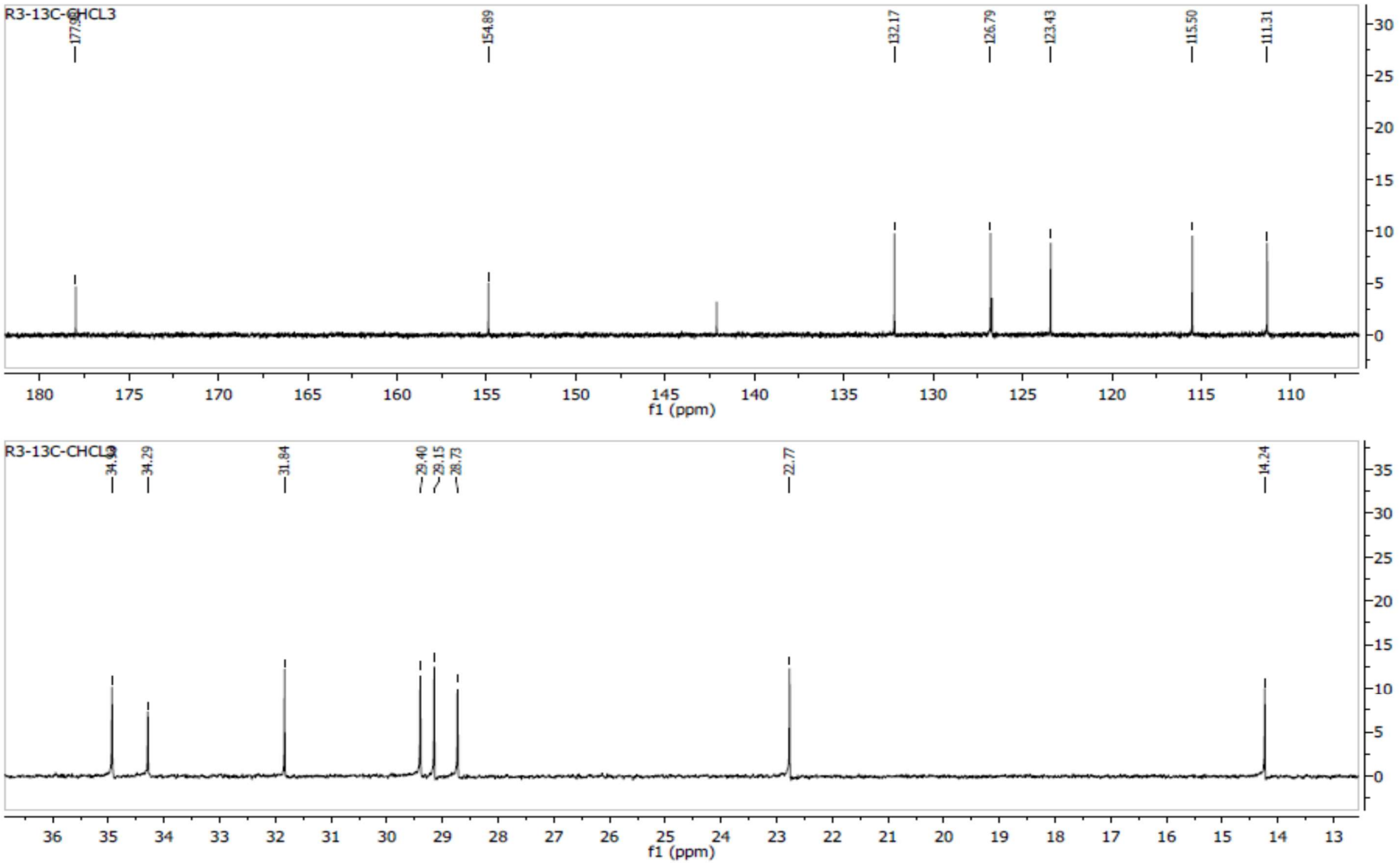

Figure S5. ^{13}C NMR spectrum of compound **1** (125 MHz, $CDCl_3$) (expanded)

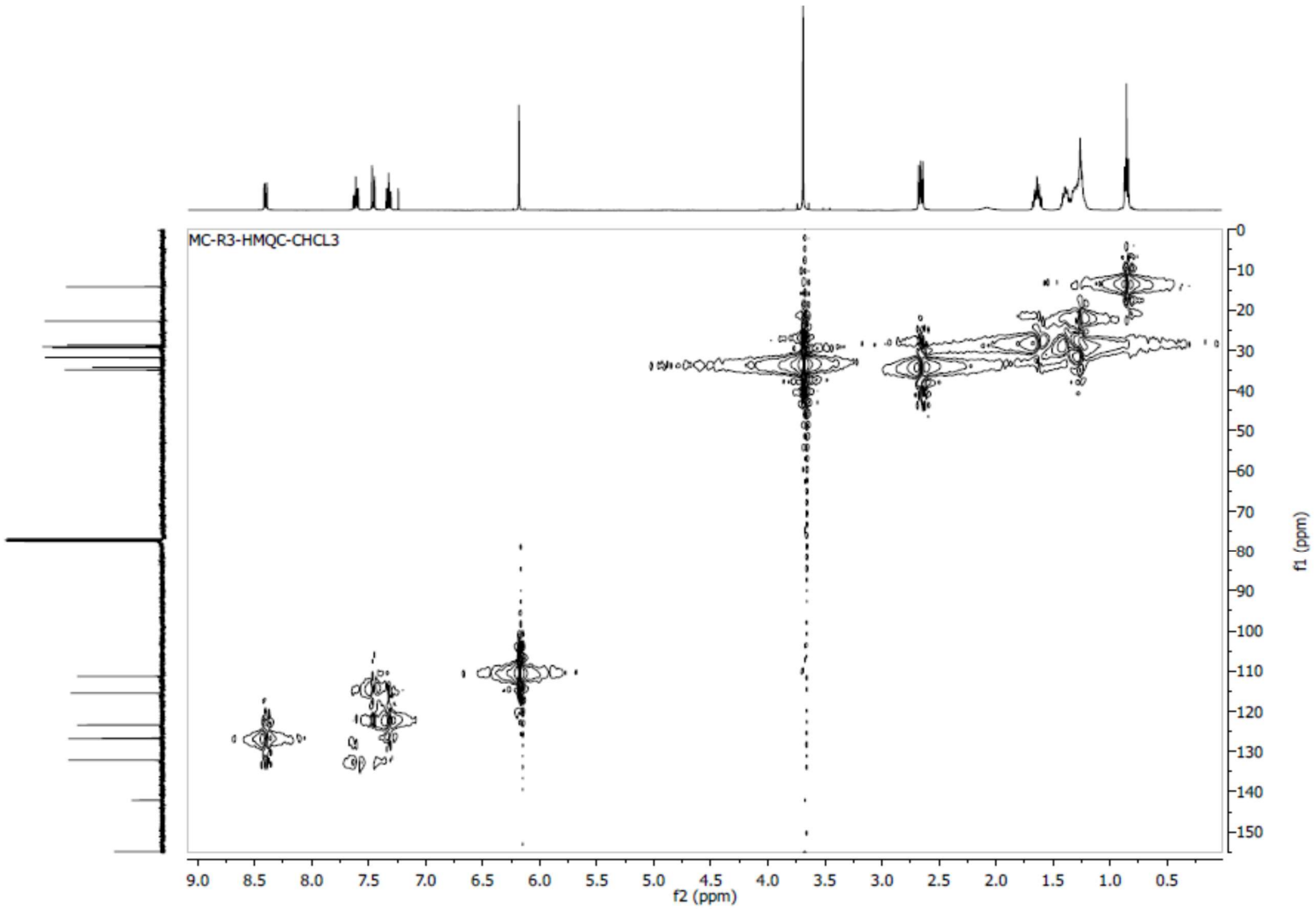

Figure S6. HMQC spectrum of compound **1**

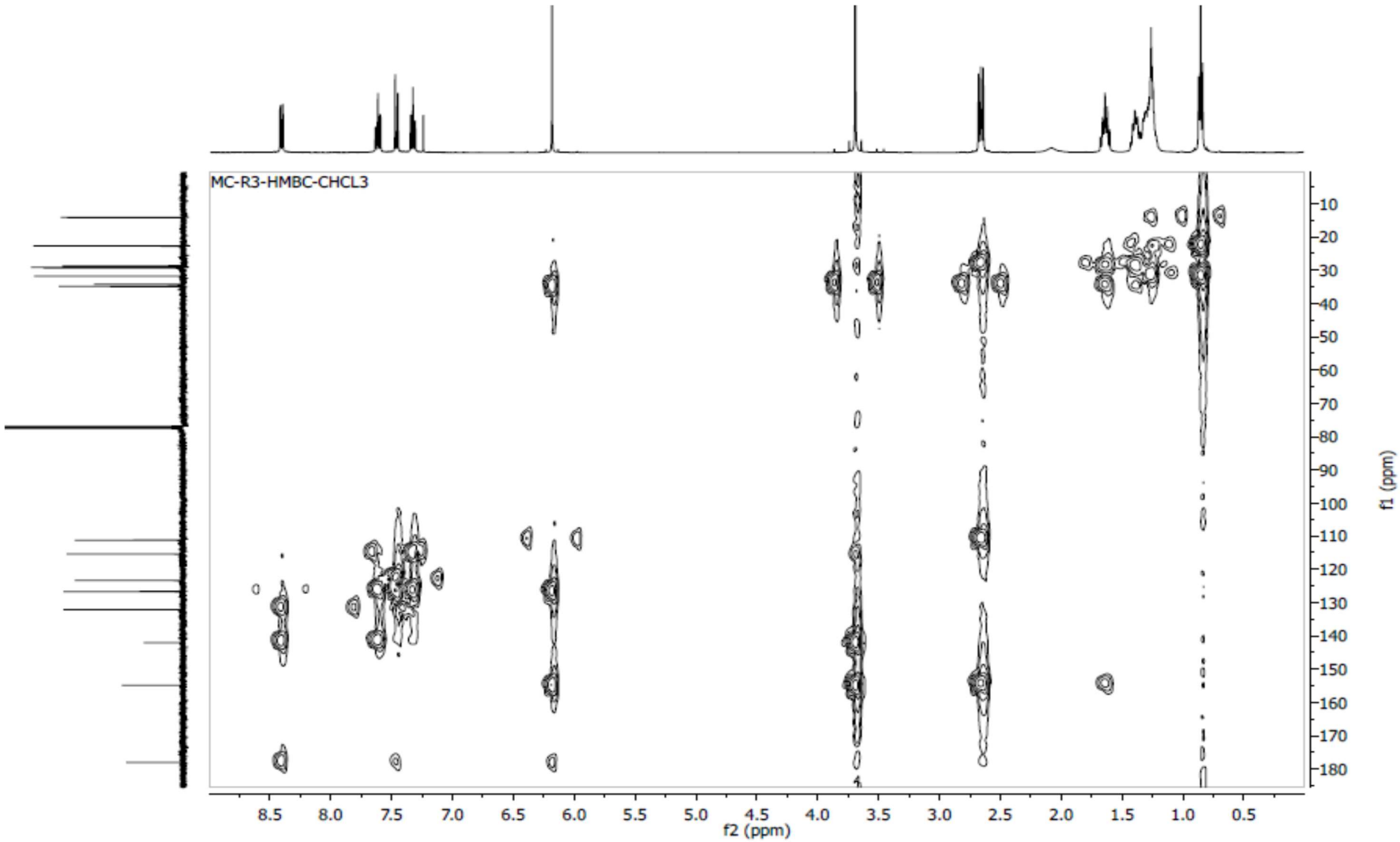

Figure S7. HMBC spectrum of compound **1**

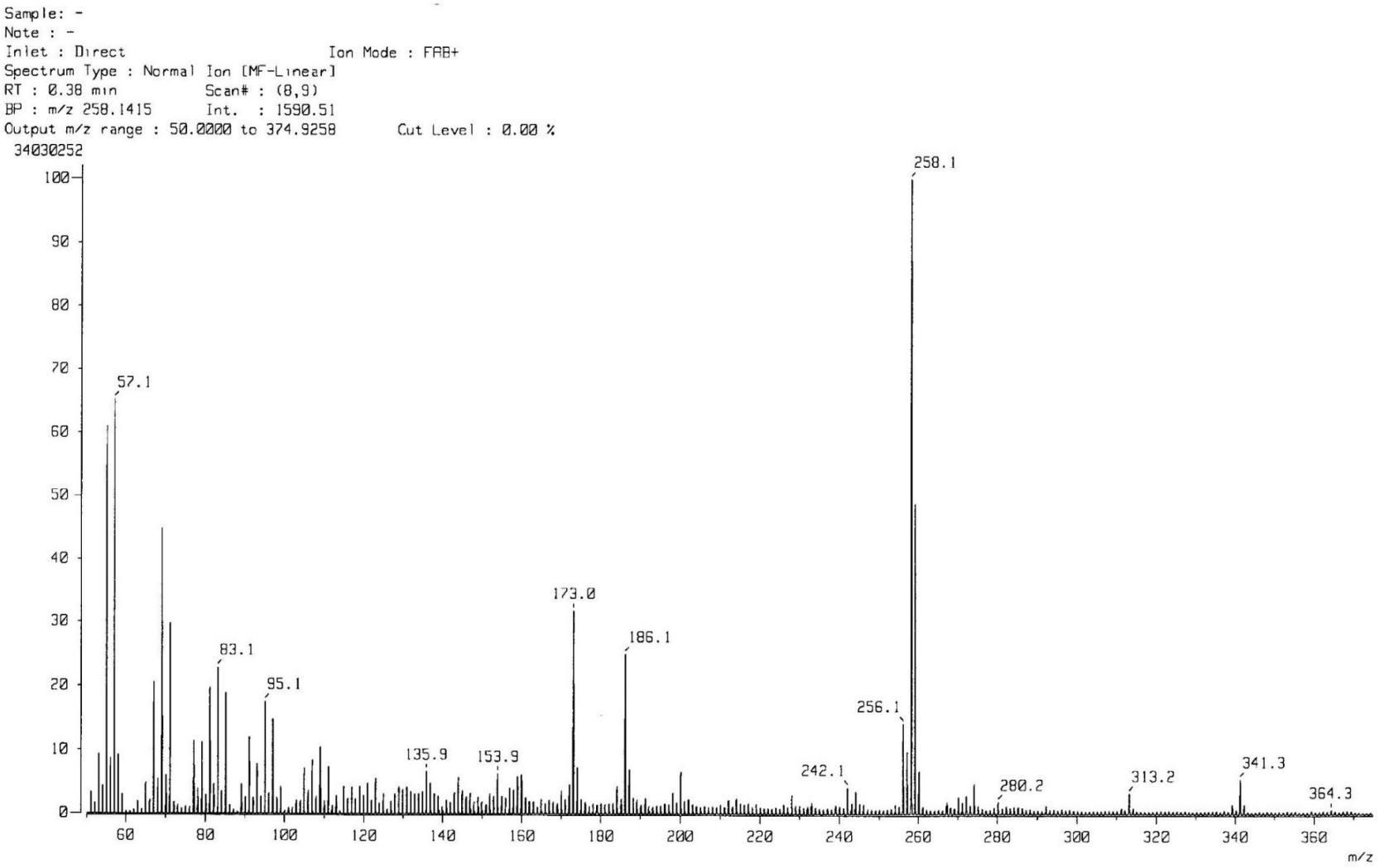

Figure S8. Mass spectrum of compound **1**

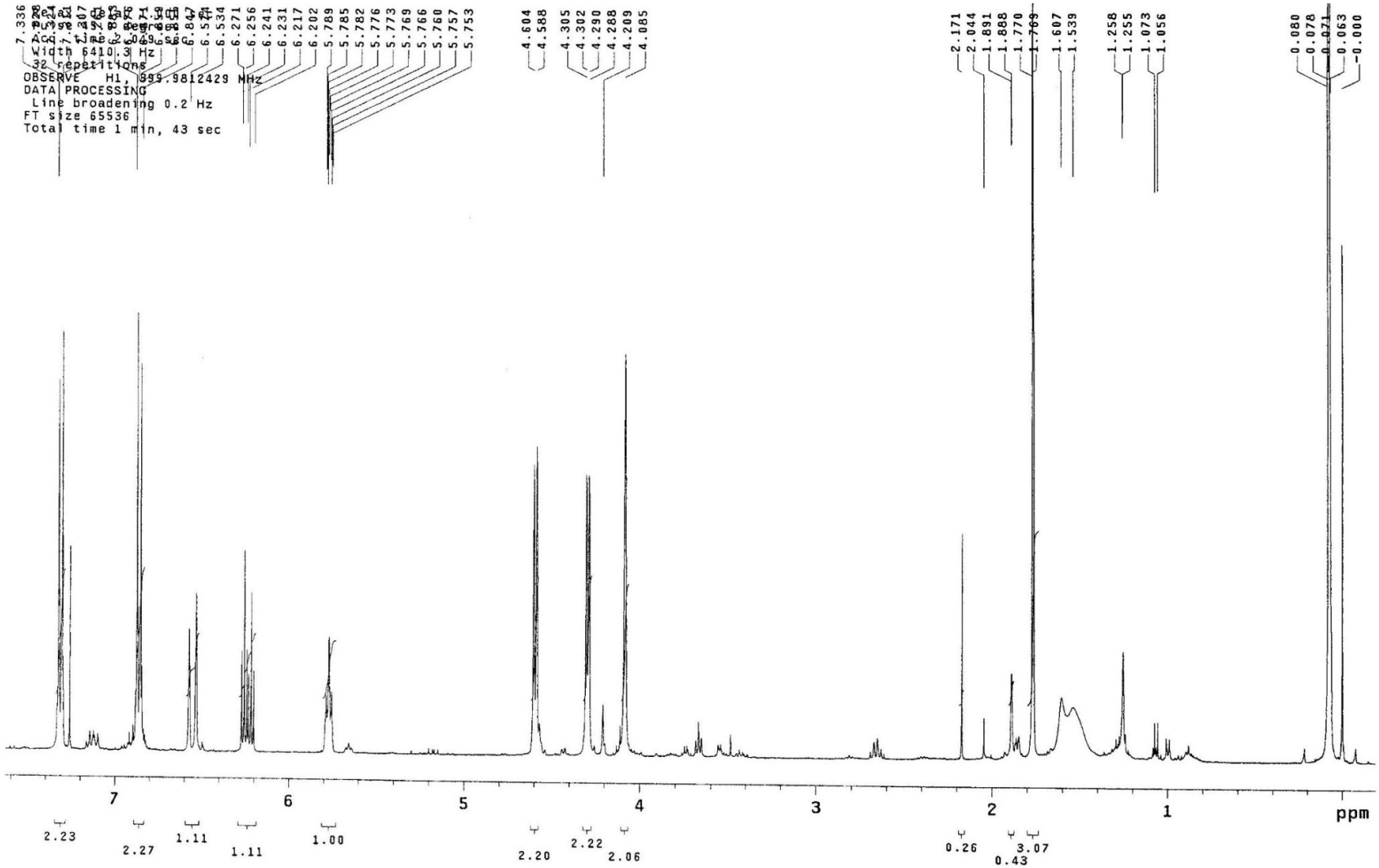

Figure S9. ^{1}H NMR spectrum of compound **2** (400 MHz, $CDCl_3$)

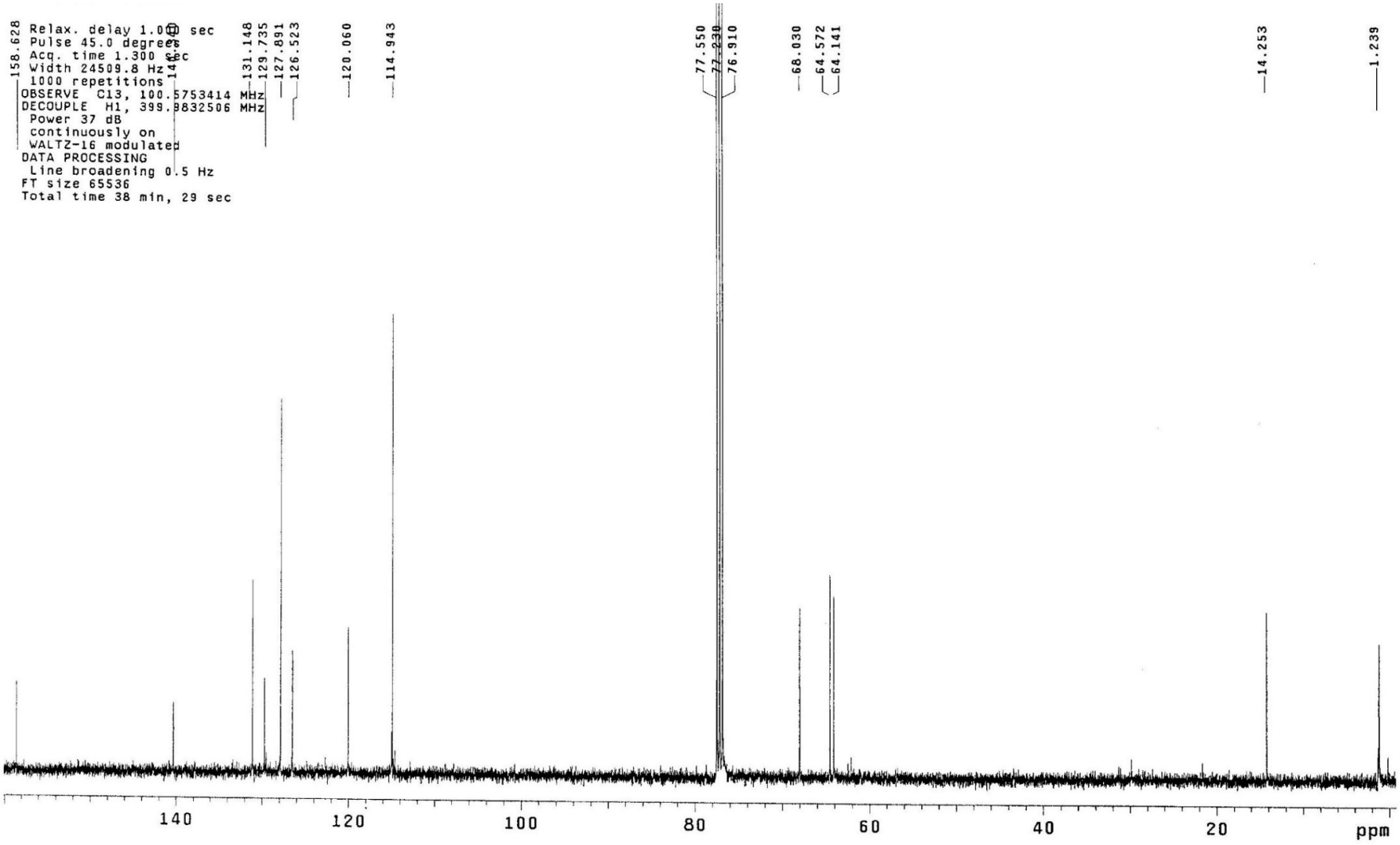

Figure S10. ^{13}C NMR spectrum of compound **2** (100 MHz, $CDCl_3$)

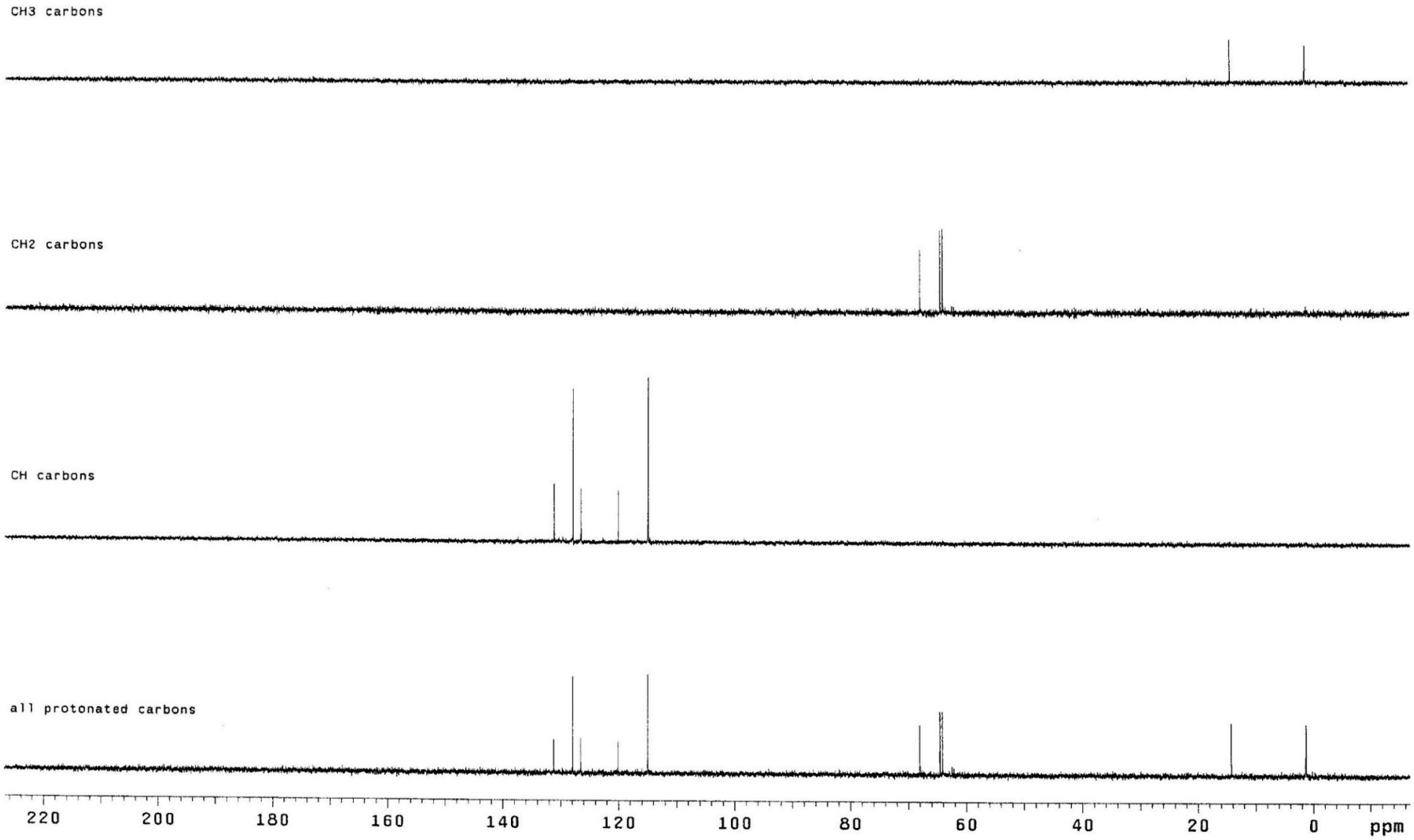

Figure S11. DEPT spectrum of compound **2**

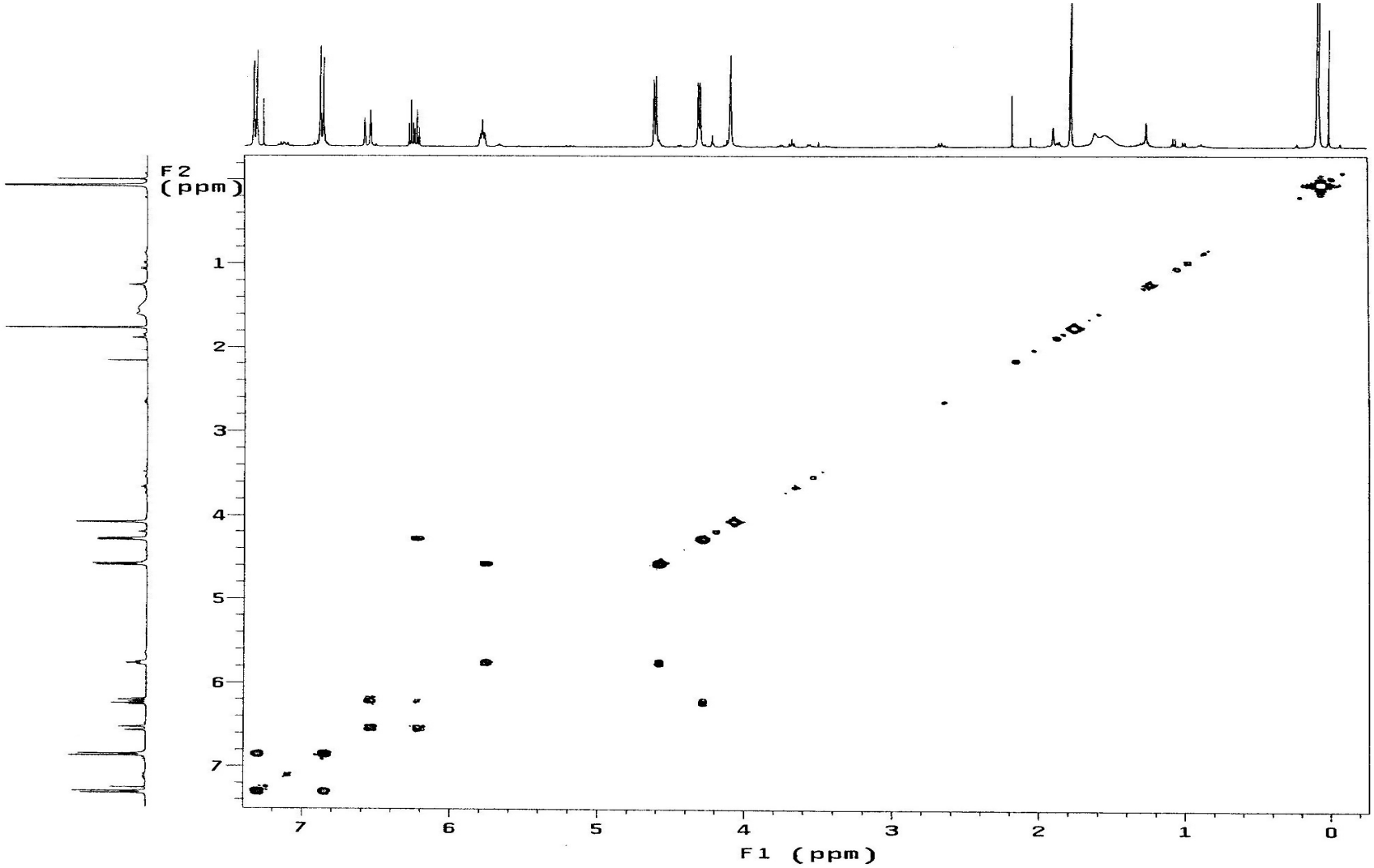

Figure S12. COSY spectrum of compound **2**

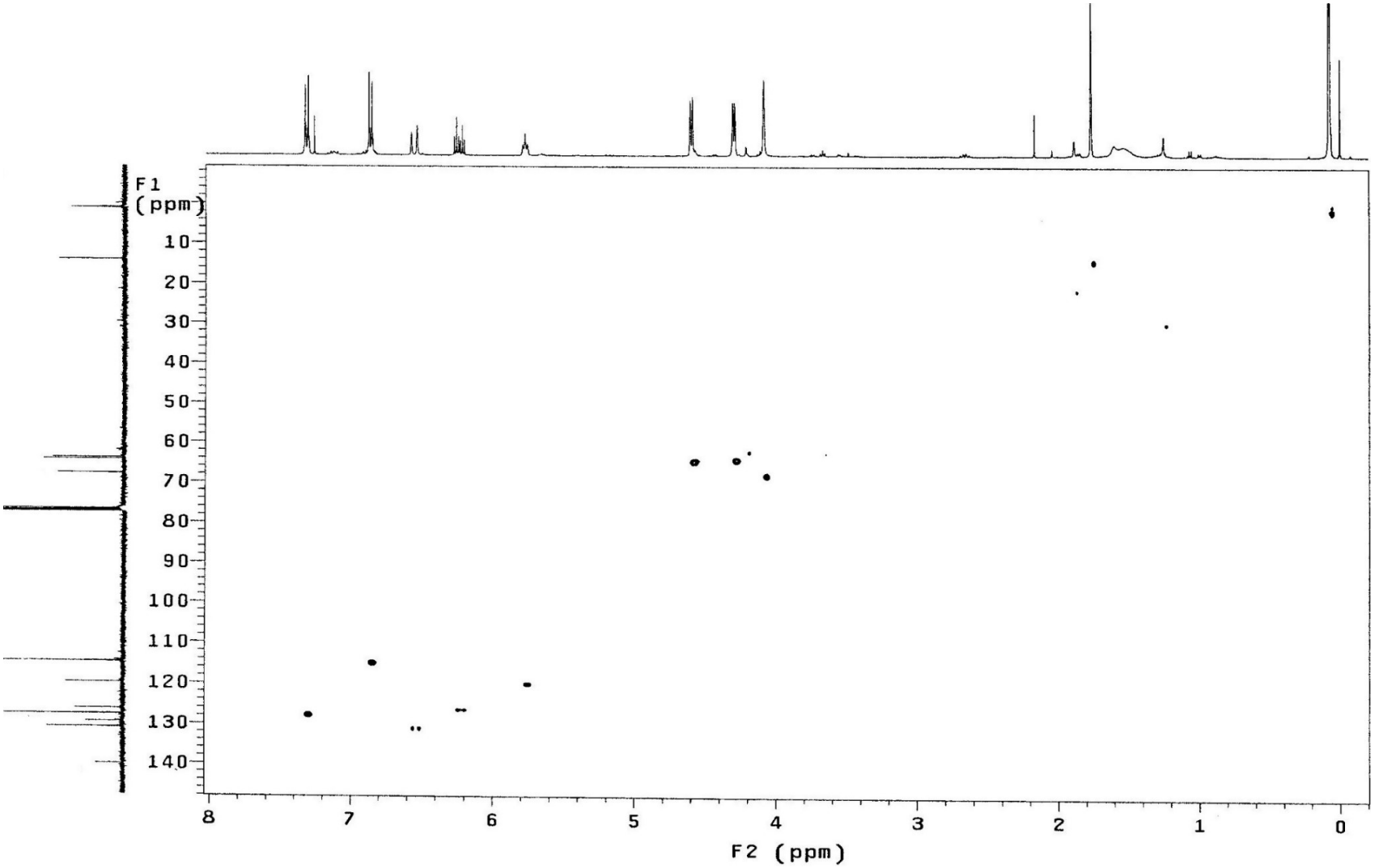

Figure S13. HSQC spectrum of compound **2**

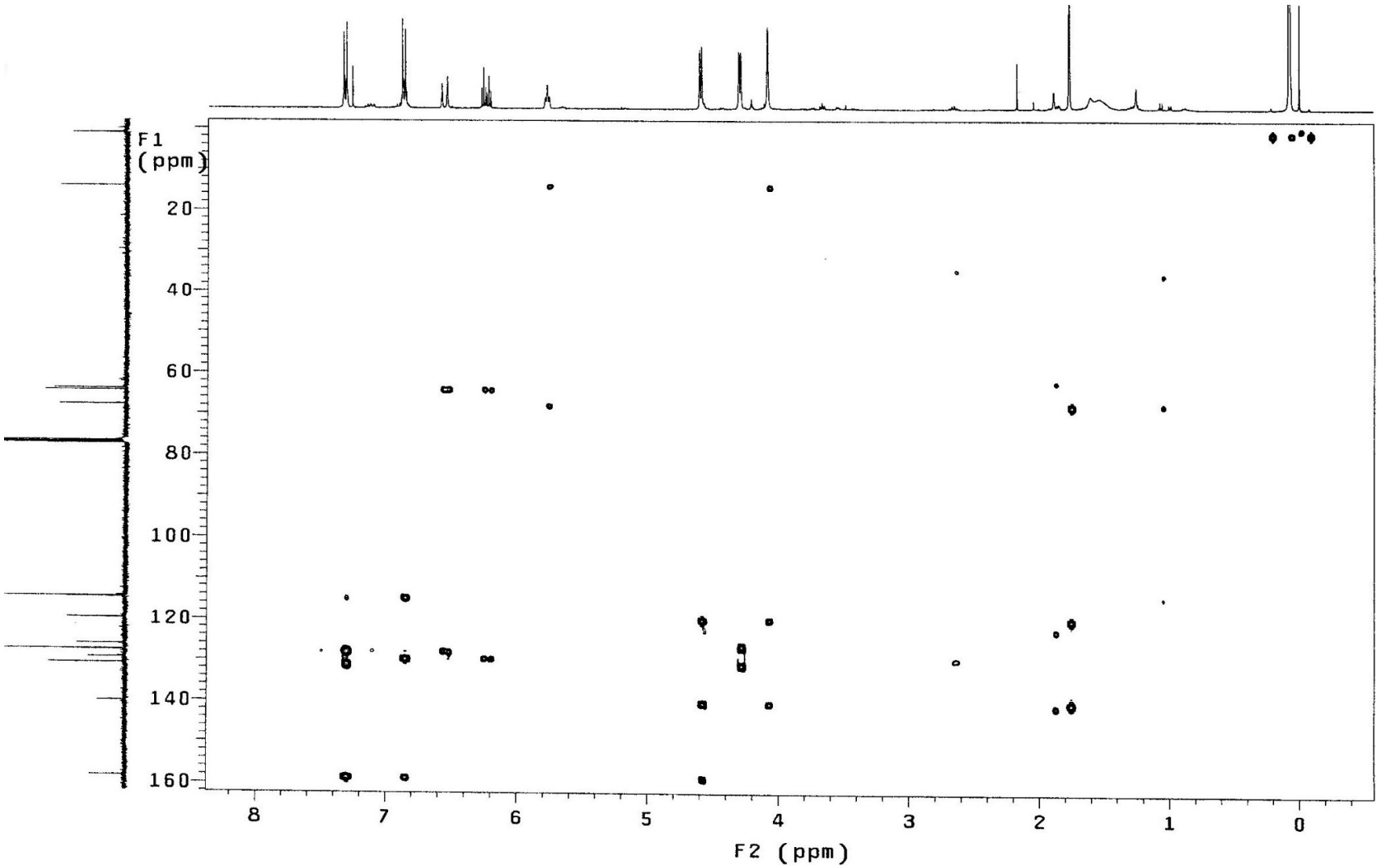

Figure S14. HMBC spectrum of compound **2**

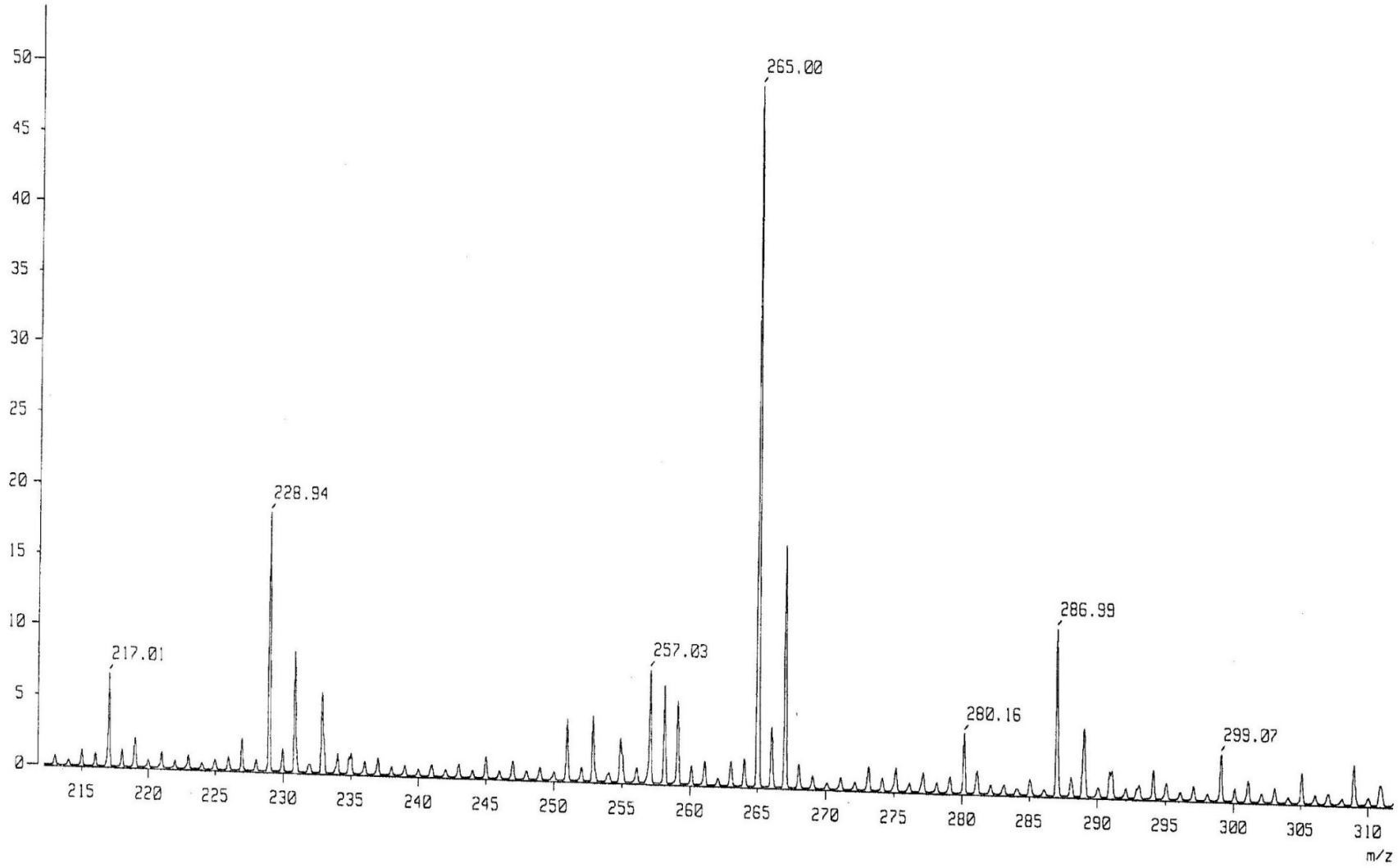

Figure S15. Mass spectrum of compound **2**

Table S1. Molecular docking simulation results for inhibitory complexes between the controlled drug voglibose (**D**) and the proteins 3W37, 3AJ7 and PTP1B

Ligand-protein complex			**Hydrogen bond**						**van der Waals interaction**
Name	**DS**	**RMSD**	**L**	**P**		**T**	**D**	**E**	
D-3W37	-14.1	1.77	O	O	Glu792	H-donor	2.94	-1.2	Thr662, Asp666, Leu663, Gly791, Tyr659, Val760, Thr790, Gly698, Asn758, Arg699, Arg676, Ile671
			O	O	Ile759	H-donor	2.79	-1.4	
			O	O	Glu792	H-donor	2.88	-1.6	
			O	O	Arg670	H-acceptor	2.91	-0.7	
D-3AJ7	-13.6	1.02	O	O	Asp352	H-donor	2.78	-1.1	Phe303, Gln279, Thr306, Phe159, Tyr158, Phe178, Glu277, Asn350, Val216, Arg315, Asp215
			O	O	Glu411	H-donor	3.15	-1.5	
			O	N	Arg4429	H-acceptor	3.07	-1.4	
			O	N	Gln353	H-acceptor	2.84	-1.5	
D-PTP1B	-14.5	1.40	O	O	Lys41	H-donor	3.00	-1.1	Asn44. Ala35, Arg45, Tyr46, Lys36, Ser50
			O	C	Lys41	H-acceptor	3.31	-0.9	
			O	N	Lys41	H-acceptor	3.17	-0.8	
			N	C	Arg47	H-acceptor	3.39	-0.8	
DS: Docking score energy (kcal.mol^{-1}); **RMSD**: Root-mean-square deviation (Å)									
L: Ligand; **P**: Protein; **T**: Type; **D**: Distance (Å); **E**: Energy (kcal.mol^{-1})									

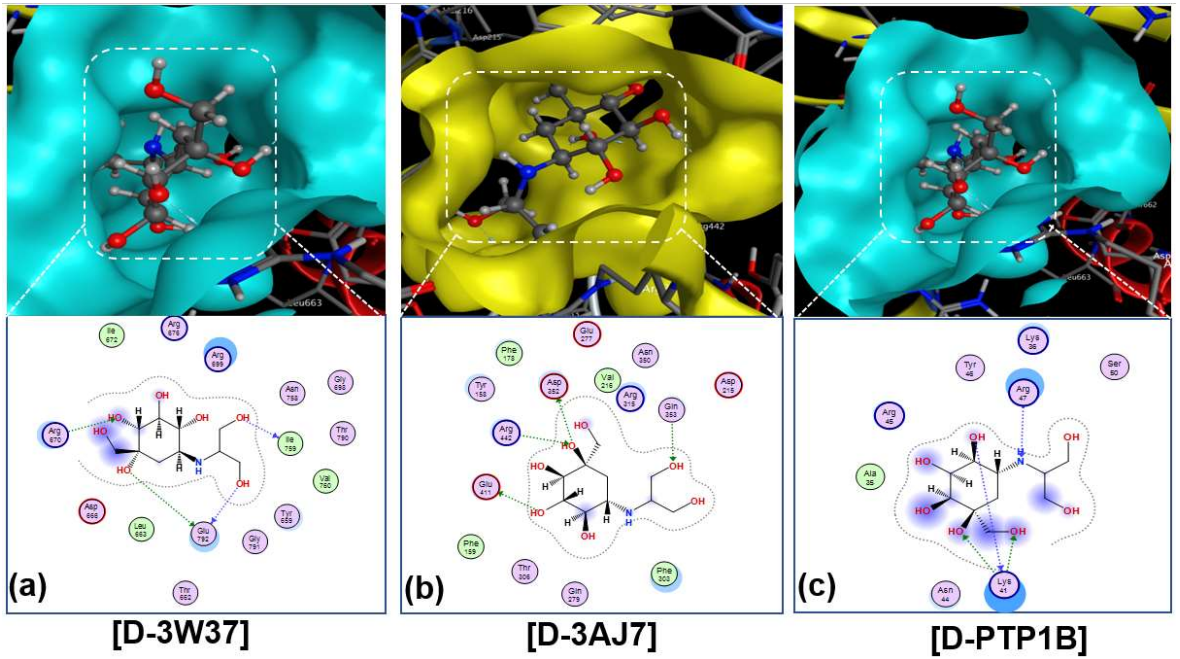

Figure S16. Visual presentation and in-pose interaction map of voglibose-protein inhibitory complexes: (a) **D-3W37**, (b) **D-3AJ7**, (c) **D-PTP1B**.

Table S2. Cartesian coordinates of the optimized **1** and **2** by DFT using basis M052X/6-311++G(d,p)

2-heptyl-1-methylquinolin-4-one (**1**)

C	5.75751200	0.41462600	0.00470900
H	6.76740300	0.79843300	0.00644600
C	5.52590100	-0.96210500	0.00402200
H	6.36091300	-1.64945800	0.00523600
C	4.24277400	-1.47241600	0.00184800
H	4.11053700	-2.54180800	0.00149900
C	3.13681700	-0.60235500	0.00026100
C	3.37134800	0.78085000	0.00096300
C	4.67850100	1.27159600	0.00318200
H	4.79439700	2.34650500	0.00365000
C	0.94521800	1.11897600	-0.00256600
H	0.09805100	1.78403100	-0.00355800
C	2.24959800	1.73918100	-0.00056800
C	0.76290300	-0.22543200	-0.00286700
N	1.83472100	-1.09420700	-0.00180700
O	2.42377400	2.94884800	-0.00029900
C	1.66846600	-2.54233500	-0.00275100
H	0.62069400	-2.80316100	-0.00489600
H	2.12844800	-2.97424900	0.88612000
H	2.13176000	-2.97335500	-0.89033800
C	-0.62306300	-0.82720200	-0.00393400
H	-0.72681900	-1.47214900	-0.88137800
H	-0.72764100	-1.47249200	0.87319100
C	-1.77766700	0.16868800	-0.00434900

H	-1.71262600	0.81474800	0.87350900
H	-1.71428100	0.81197700	-0.88439600
C	-3.12329700	-0.55272000	-0.00147500
H	-3.18870900	-1.20742500	-0.87618300
H	-3.18855400	-1.19961600	0.87905700
C	-4.30654200	0.41037900	-0.00573100
H	-4.24100800	1.06864200	0.86578400
H	-4.24609700	1.05457300	-0.88807200
C	-5.65212800	-0.30873500	0.00415500
H	-5.71632500	-0.97030000	-0.86561000
H	-5.71313800	-0.95118300	0.88837900
C	-6.84008100	0.64910900	-0.00421200
H	-6.77319500	1.31121800	0.86286900
H	-6.77984600	1.28762700	-0.88930700
C	-8.17726400	-0.08619300	0.01078000
H	-8.26469800	-0.70951800	0.90214000
H	-8.26989700	-0.73650200	-0.86052400
H	-9.01657000	0.60865200	0.00261500

3-[4-(4- methylhydroxy-2-butenyloxy)-phenyl]-2-propanol (**2**)

C	-1.16373800	0.17457300	0.81611900
H	-1.65379000	0.91735200	1.42990800
C	-1.82917900	-0.35946500	-0.28758700
C	-1.13692600	-1.27840400	-1.08166800
H	-1.62357200	-1.69843400	-1.95245000

C	0.15469700	-1.66712900	-0.77532000
H	0.69084700	-2.38384600	-1.38149200
C	0.79504600	-1.13694600	0.34437200
C	0.13203900	-0.20192400	1.13776300
H	0.61800000	0.24744700	1.98950800
O	2.05898600	-1.58561500	0.56614500
C	-3.20714700	0.00270500	-0.64521200
H	-3.51676800	-0.29573300	-1.64309300
C	-4.09505700	0.63104900	0.12420600
H	-3.85558300	0.91441200	1.14351600
C	-5.48565400	0.95386100	-0.32444200
H	-5.63838400	0.60122600	-1.34934000
H	-5.65374100	2.03038800	-0.30899600
O	-6.45769300	0.40980900	0.56140500
H	-6.28111800	-0.52982200	0.63290300
C	2.84263300	-0.95844700	1.58538800
H	3.74339700	-1.56755200	1.63068800
H	2.33188000	-1.05129500	2.54573700
C	3.16598400	0.48795600	1.29956500
H	3.00742500	1.18421600	2.11669700
C	3.60428500	0.96285000	0.13471000
C	3.81880800	0.09463500	-1.08179300
H	3.90402400	-0.95748800	-0.81463500
H	4.73464200	0.40403200	-1.58544100
C	3.83135700	2.42739000	-0.09851300
H	4.88228900	2.61654100	-0.32908200

H	3.54723900	3.02615600	0.76467400
H	3.24724800	2.74402400	-0.96394300
O	2.77398800	0.29717600	-2.02777100
H	1.95083300	0.03119600	-1.60892000

Table S3. PTP1B and α-glucosidase inhibitory activities of total methanol extracts and its fractions from *T. ruticarpum*

Compounds	PTP1B	α-glucosidase
	% Inhibition, μg/mL[a]	**% Inhibition, μg/mL[a]**
MeOH extract	53.2 ± 1.8	ND[b]
EtOAc fraction	67.7 ± 2.3	-
H_2O fraction	23.5 ± 0.6	-
TR1	-[b]	47.9 ± 1.3
TR2	-	57.5 ± 2.7
TR3	-	< 20
TR4	-	< 20
TR5	-	27.3 ± 2.4
TR6	-	43.6 ± 2.1
TR7	-	< 20
TR8	-	< 20
TR9	-	44.8 ± 3.2
TR10	-	52.6 ± 2.9

[a] Results are expressed as % inhibition with the final tested concentration of 30 μg/mL for the testing sample (n = 2).

[b] Data not determined.