Supplementary Material

Anatolicin, a Highly Potent and Selective Cytotoxic Sesquiterpene Coumarin, from the Root Extract of *Heptaptera anatolica*

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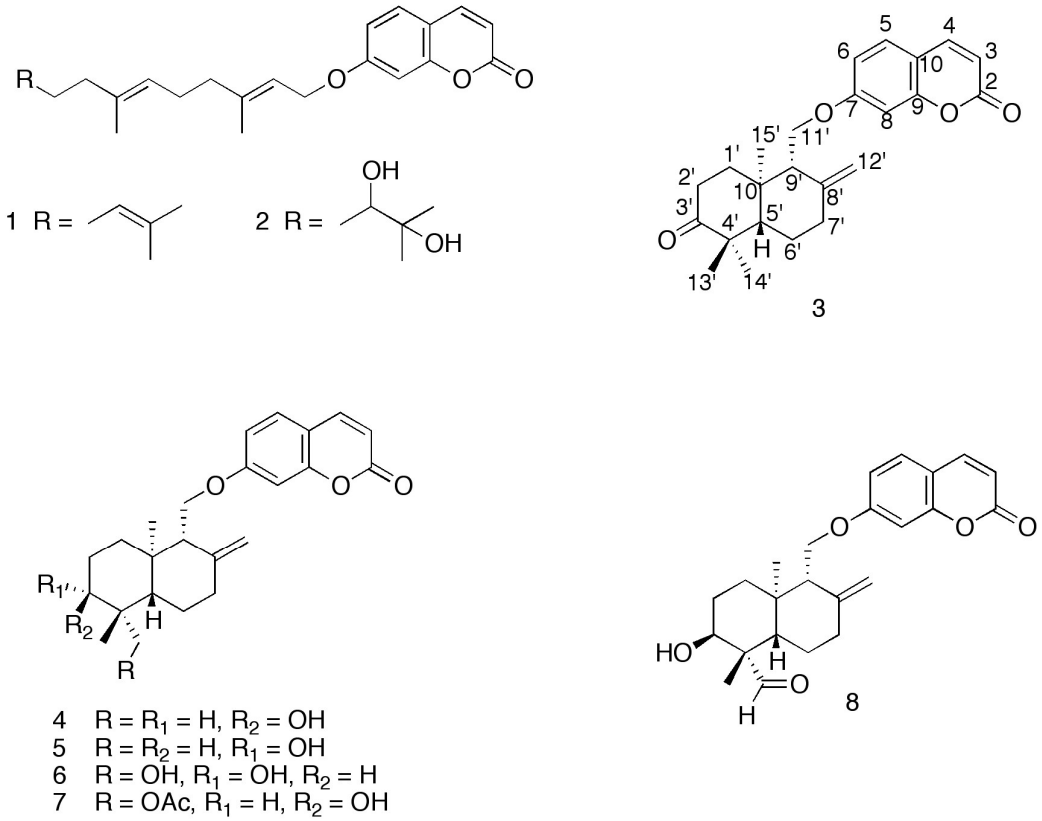


Fig. S1 Structures of sesquiterpene coumarins isolated from the root extract of *Heptaptera anatolica*.

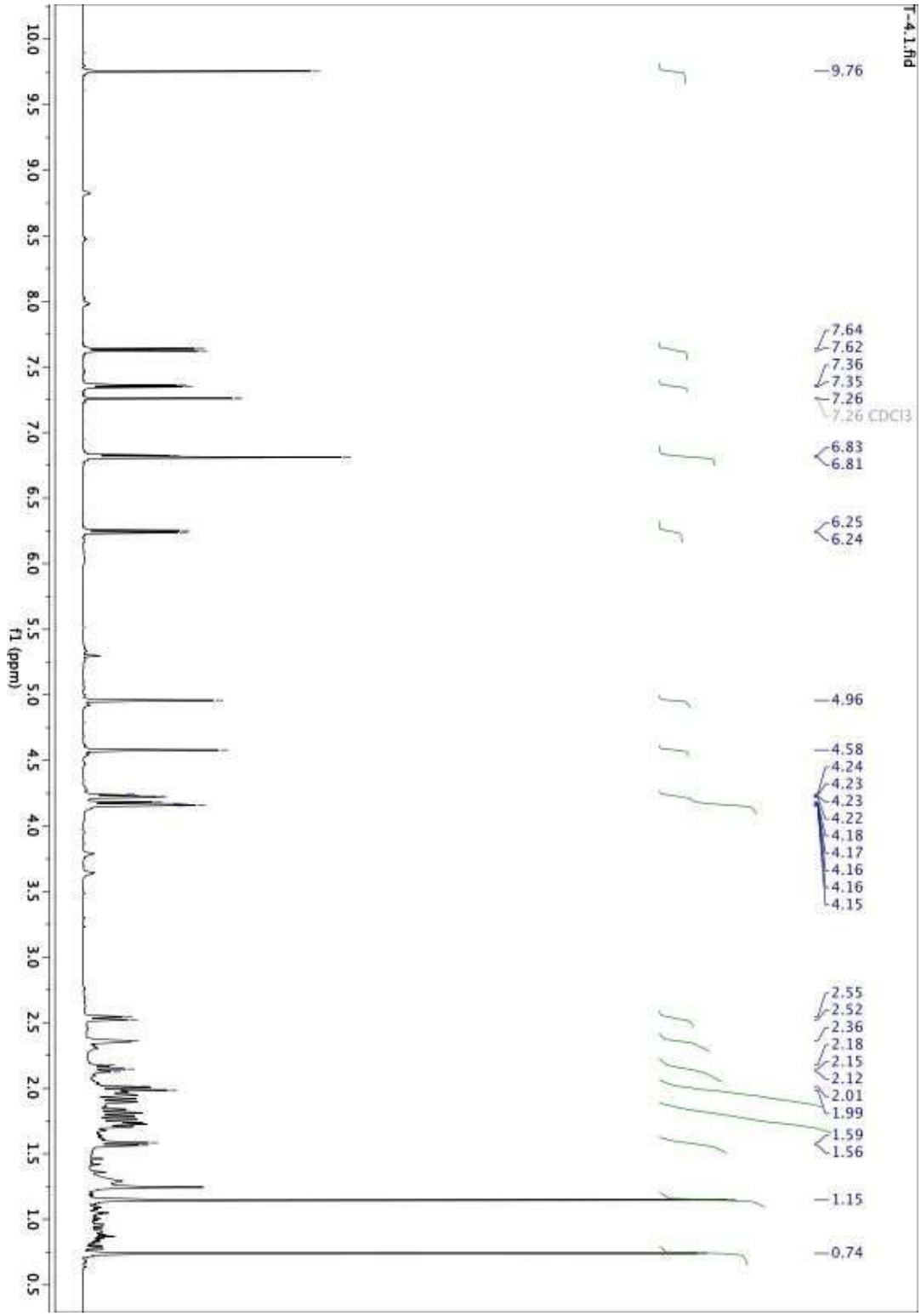


Fig. S2 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of anatolicin (**8**)

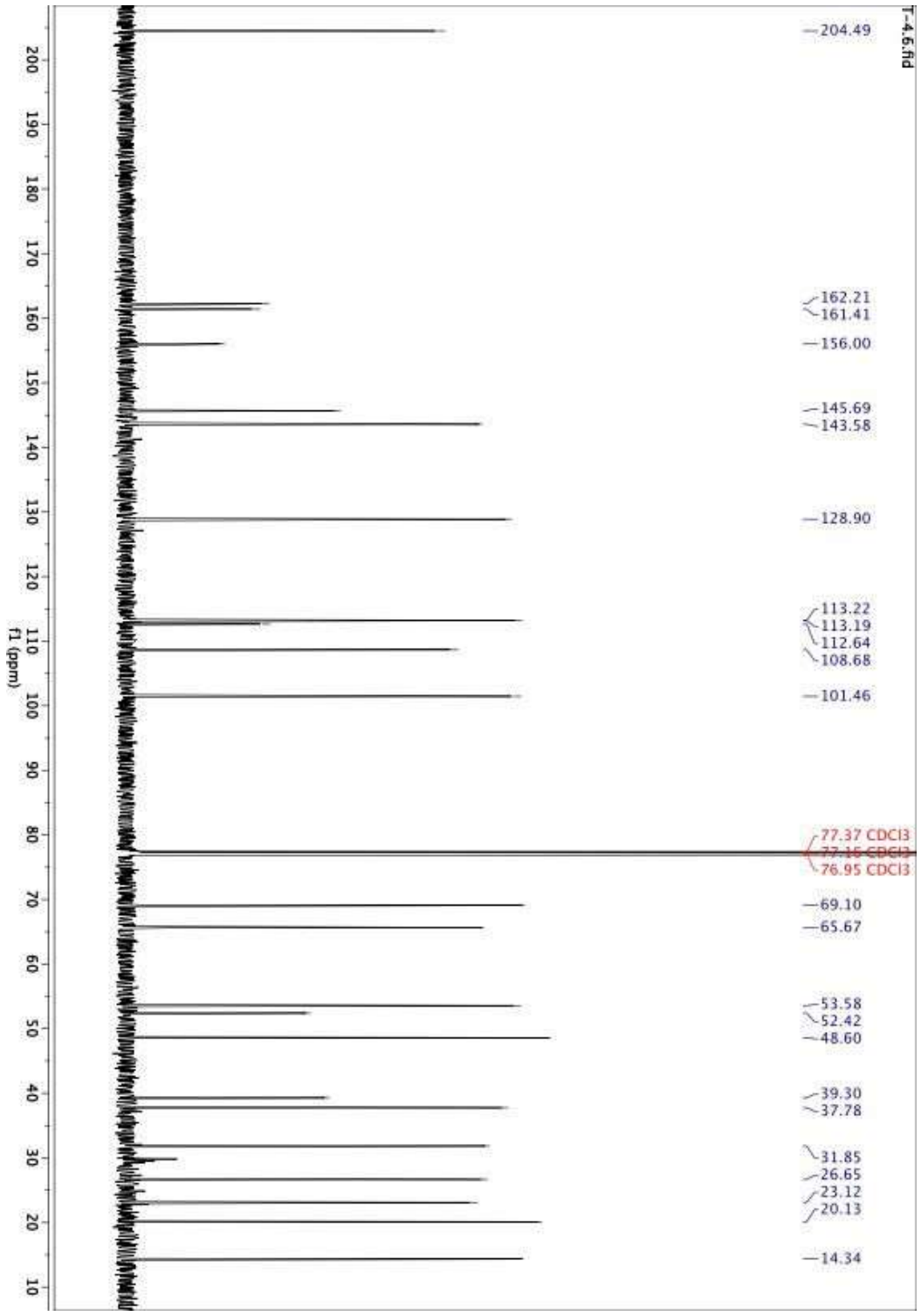


Fig. S3 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of anatolicin (**8**)

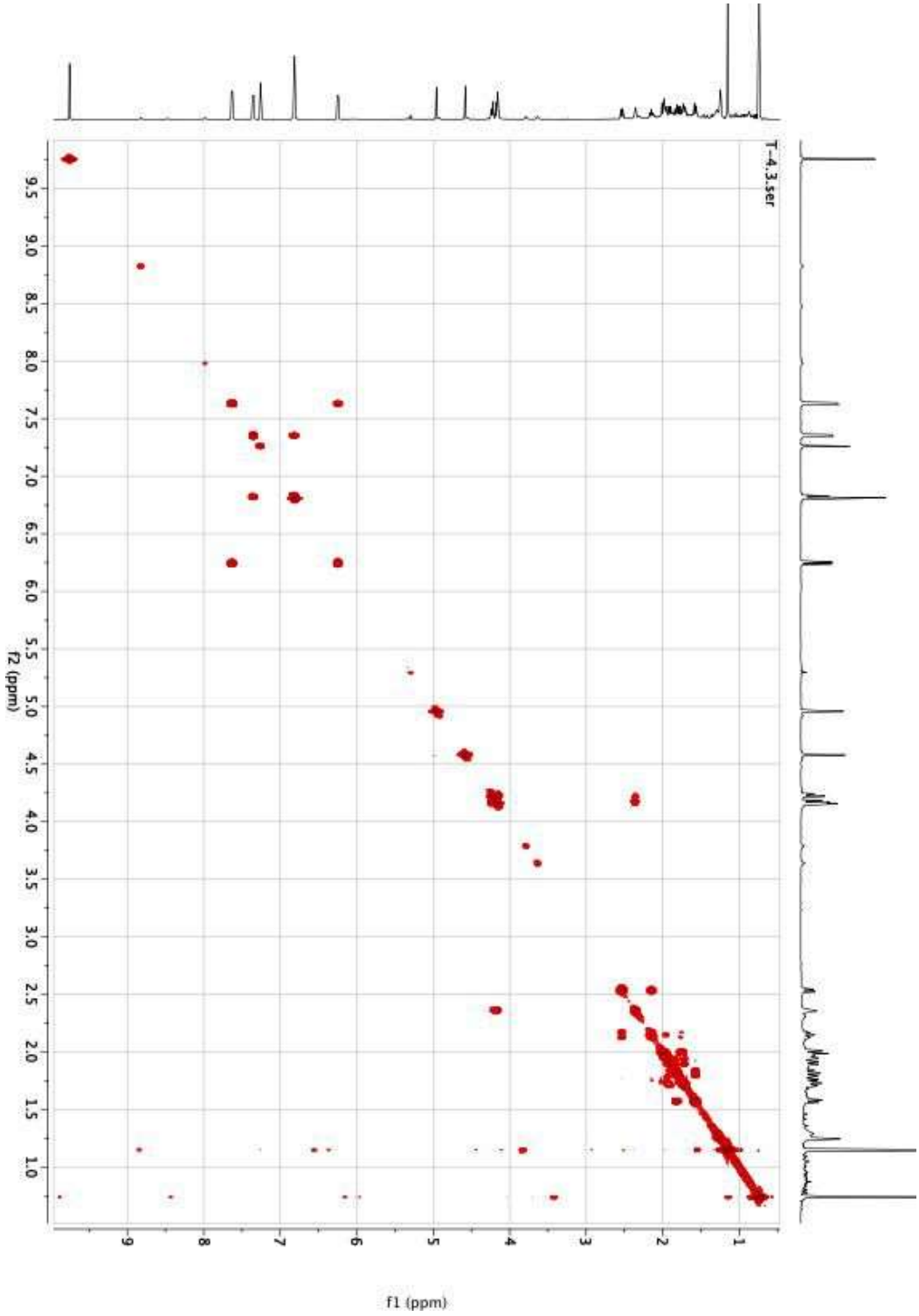


Fig. S4 2D COSY spectrum of anatolicin (**8**)

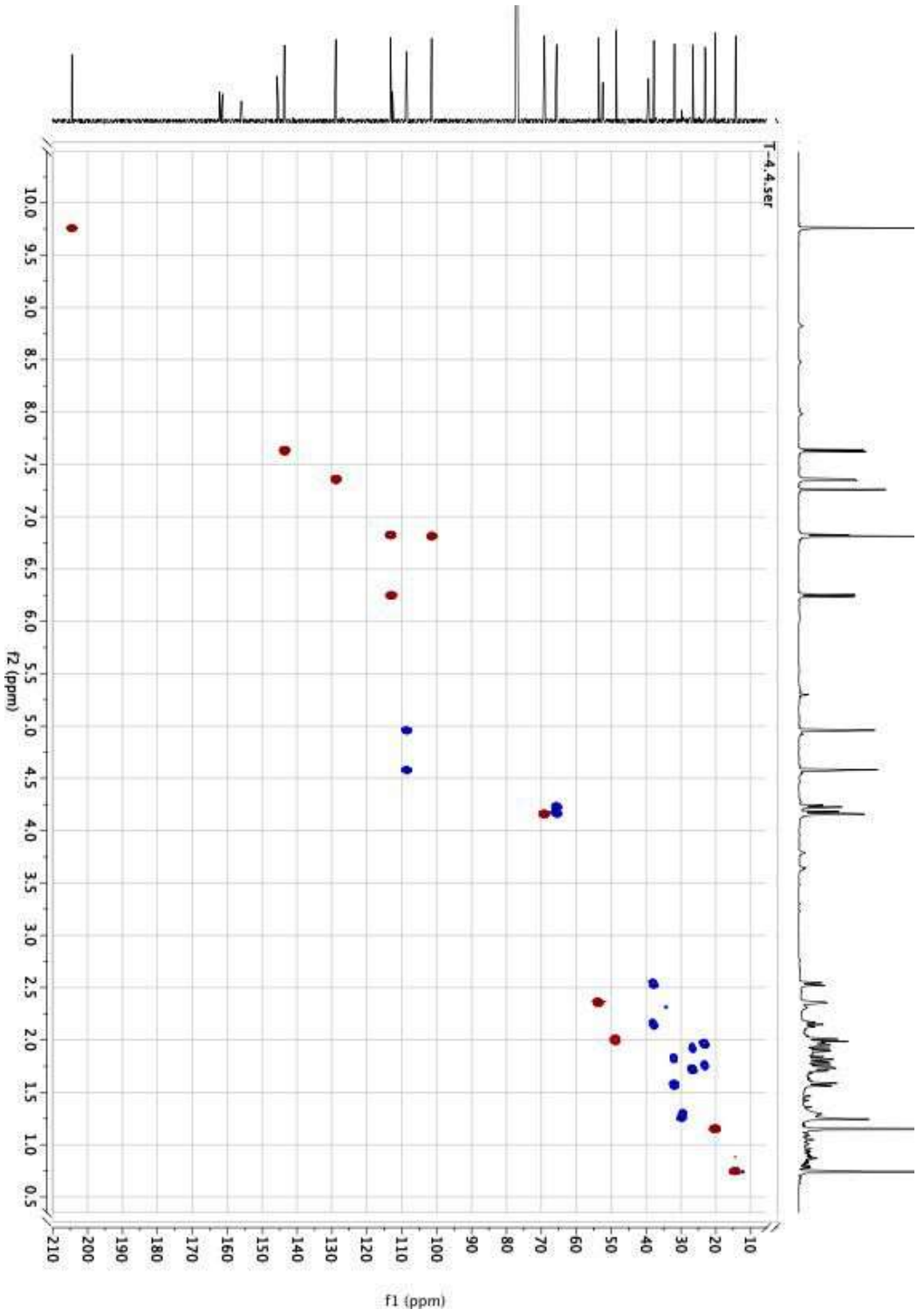


Fig. S5 2D HSQC spectrum of anatolicin (**8**)

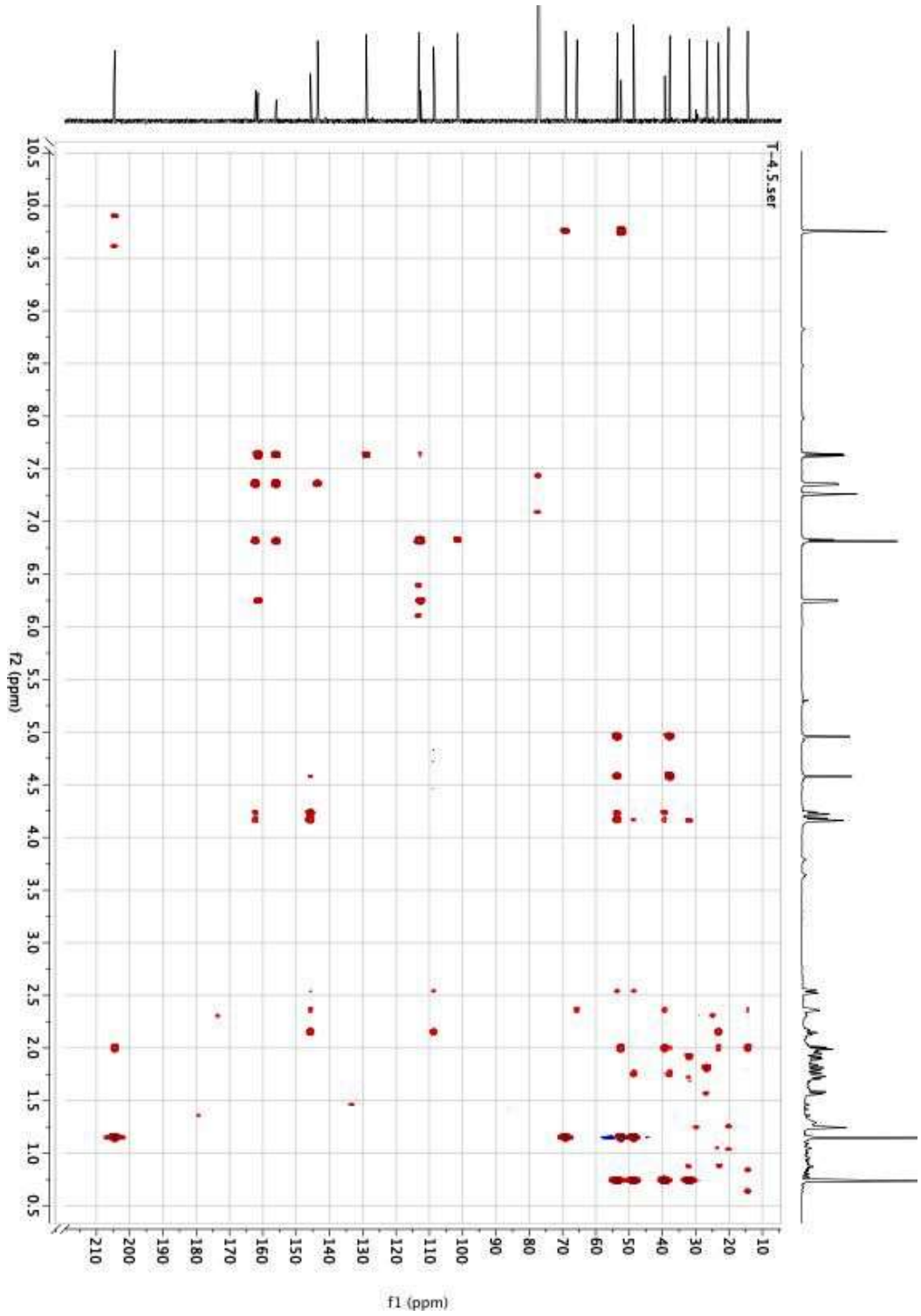


Fig. S6 2D HMBC spectrum of anatolicin (**8**)

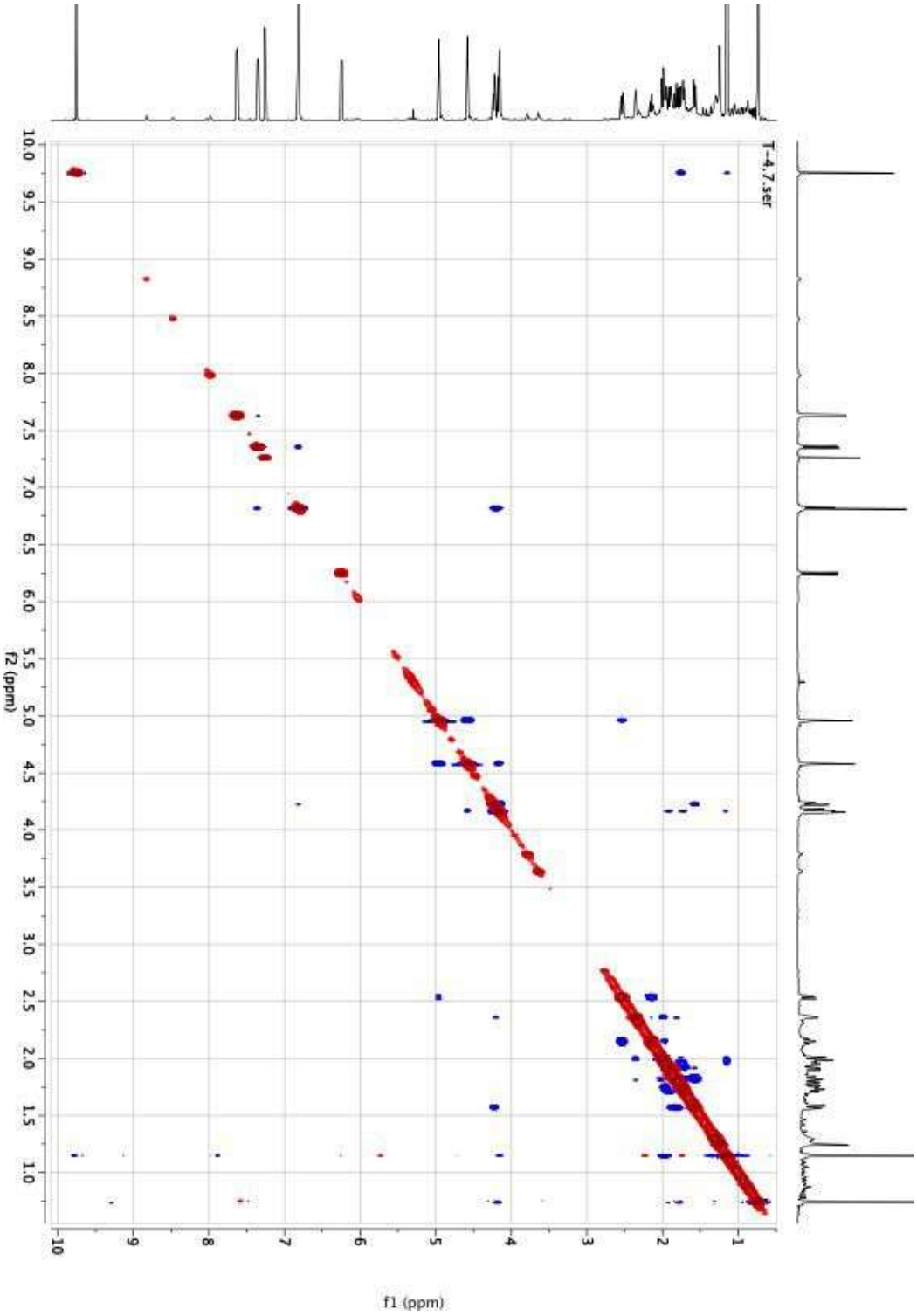


Fig. S7 2D NOESY spectrum of anatolicin (**8**)

Qualitative Compound Report

Data File	101I069F.d	**Sample Name**	101I069F
Sample Type	Sample	**Position**	Vial 41
Instrument Name	Instrument 1	**User Name**	Heidi
Acq Method	SMaccms_DESI(+)_Centroid.m	**Acquired Time**	1/15/2018 11:21:35 AM
IRM Calibration Status	Success	**DA Method**	Heidi.m
Comment			

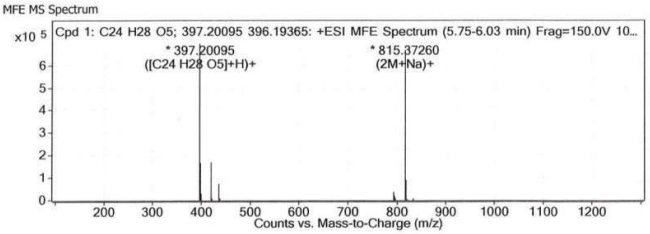
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

Compound Table

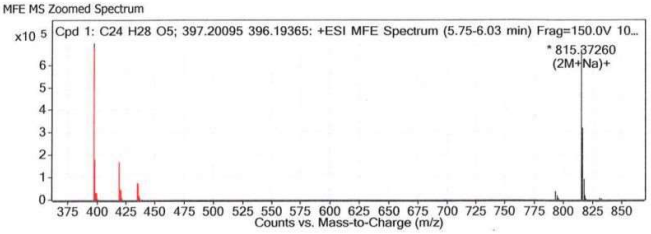
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C24 H28 O5; 397.20095 396.19365	5.81	396.19365	C24 H28 O5	C24 H28 O5	0.05	C24 H28 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H28 O5; 397.20095 396.19365	397.20095	5.81	Find by Molecular Feature	396.19365

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
397.20095	1	695393.69	C24 H28 O5	(M+H)+
398.20425	1	164220.08	C24 H28 O5	(M+H)+
399.20696	1	26898.86	C24 H28 O5	(M+H)+
419.18266	1	169149.11	C24 H28 O5	(M+Na)+
420.18617	1	41114.52	C24 H28 O5	(M+Na)+
435.15636	1	72662.35	C24 H28 O5	(M+K)+

Fig. S8 HRESIMS spectrum of anatolicin (**8**)

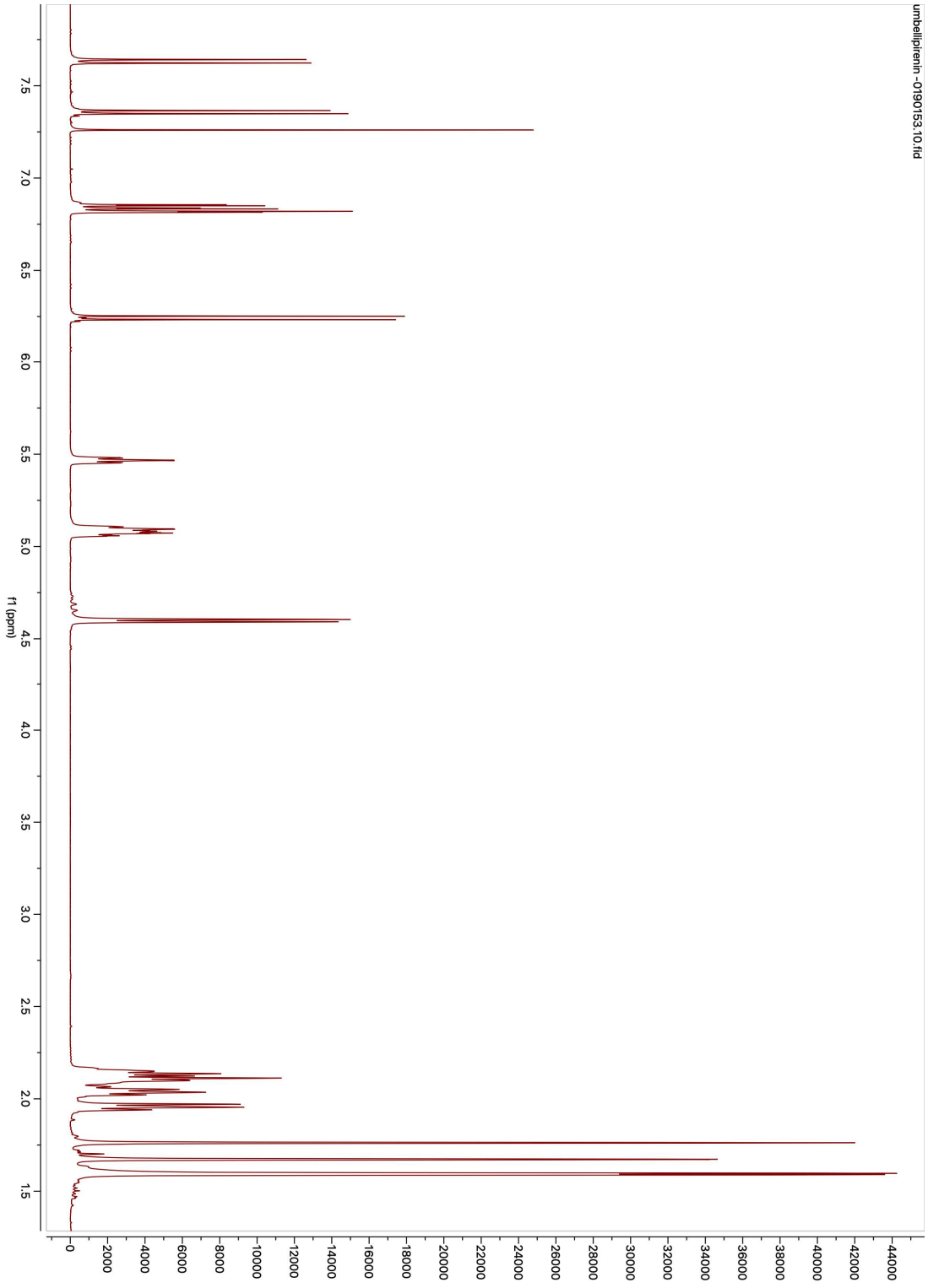


Fig. S9 ^{1}H NMR spectrum of Umbelliprenin (**1**)

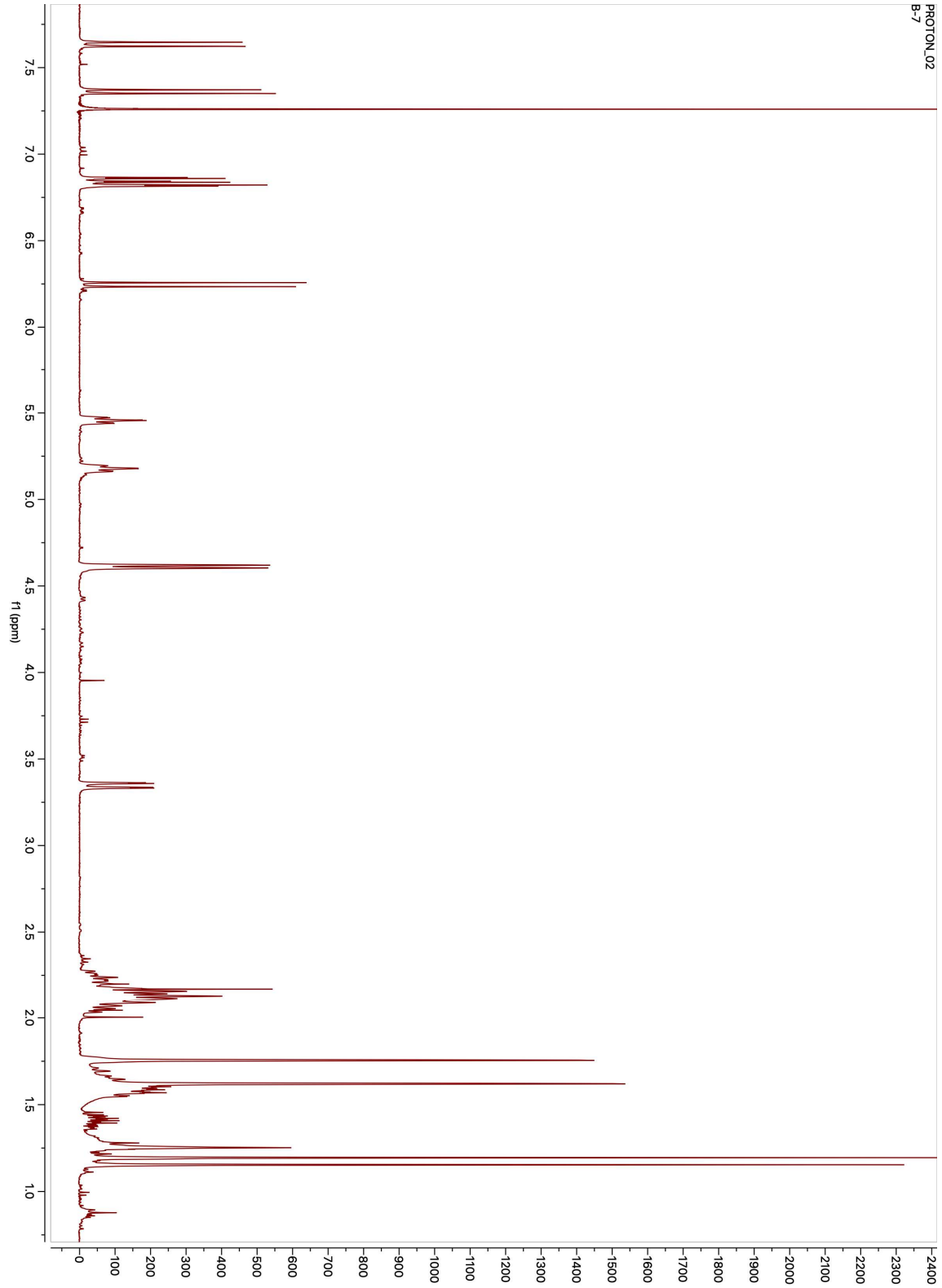


Fig. S10 ^{1}H NMR spectrum of Karatavicinol (**2**)

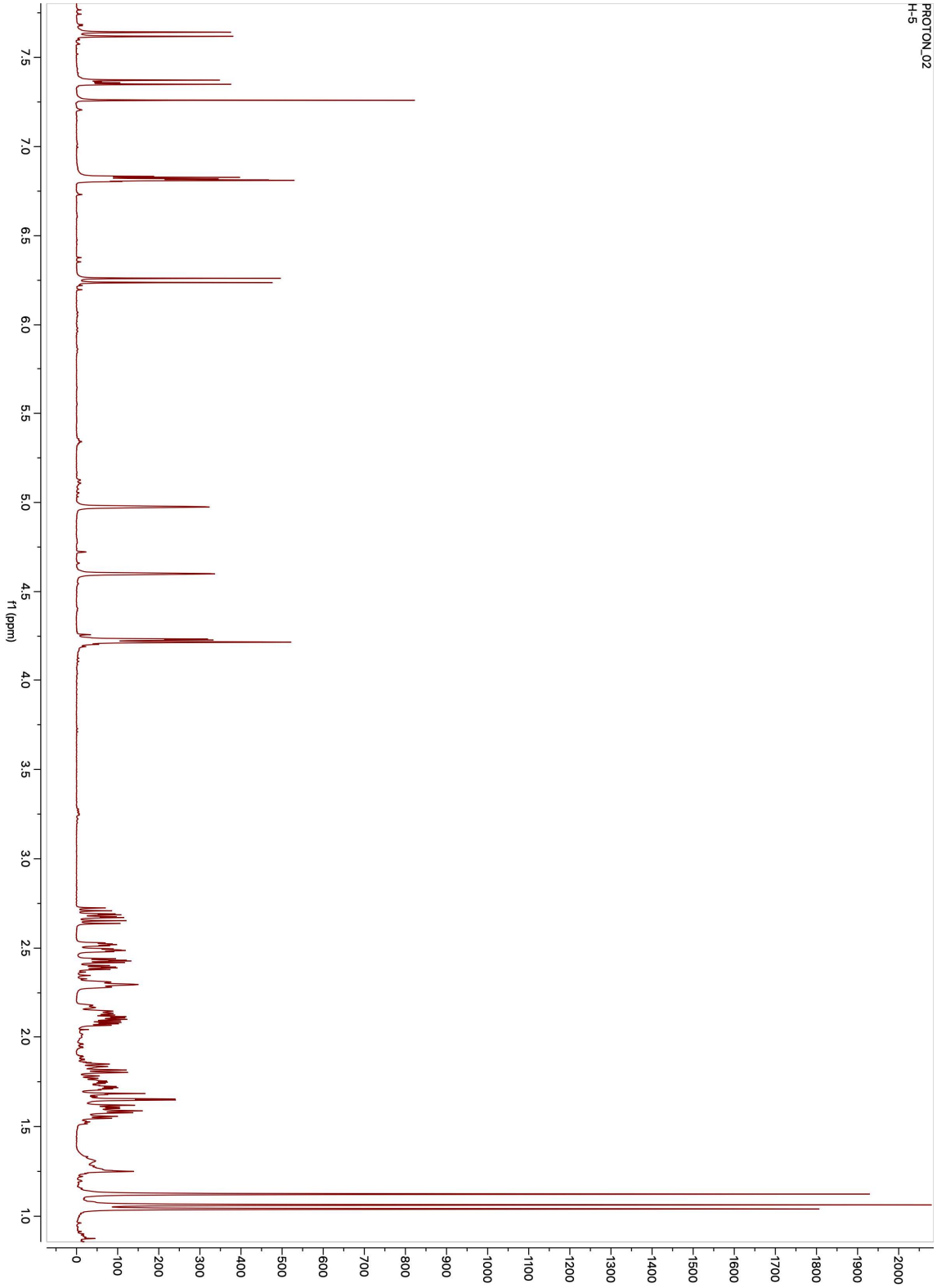


Fig. S11 ^{1}H NMR spectrum of Badrakemone (**3**)

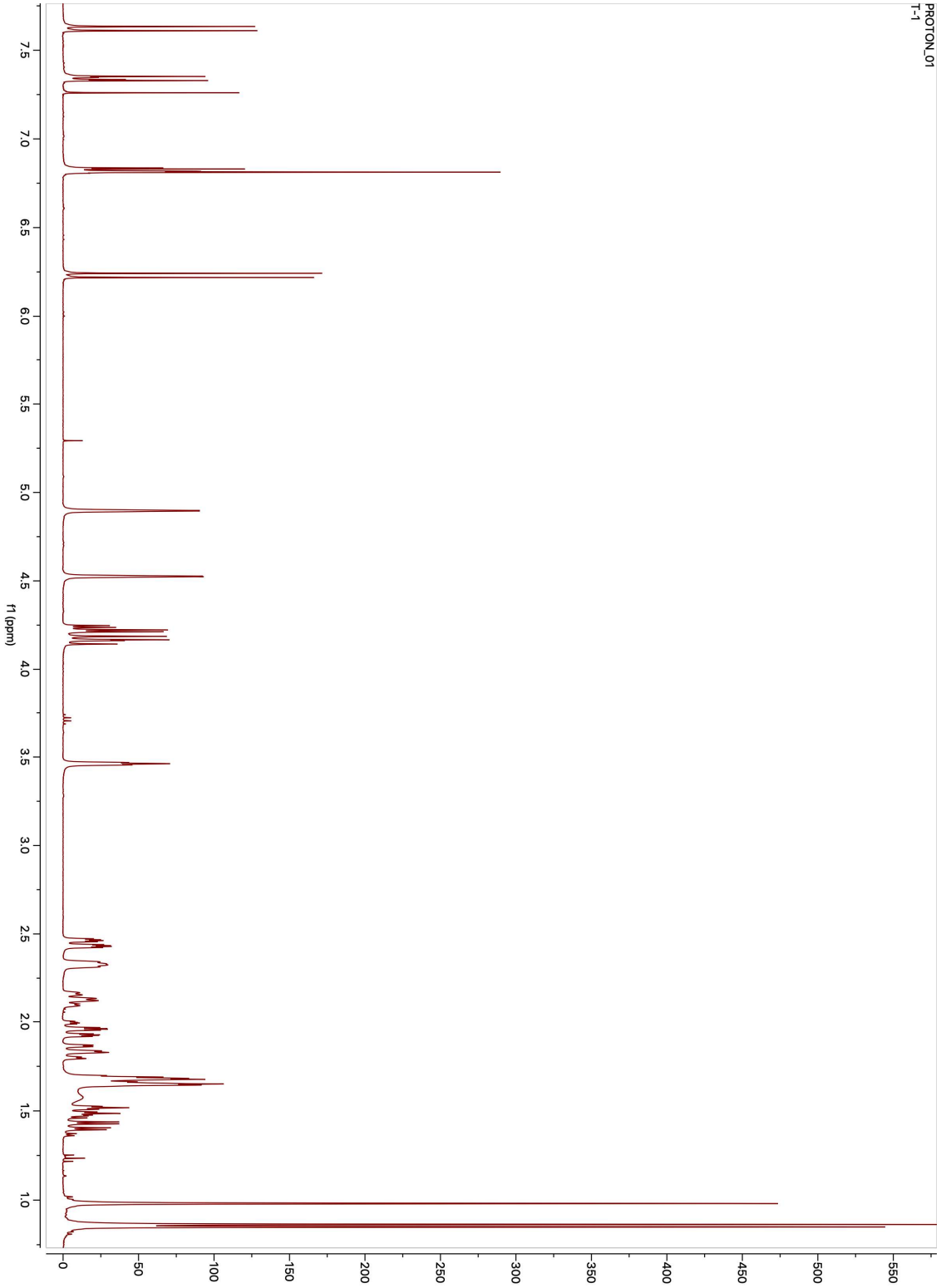


Fig. S12 ^{1}H NMR spectrum of Badrakemin (**4**)

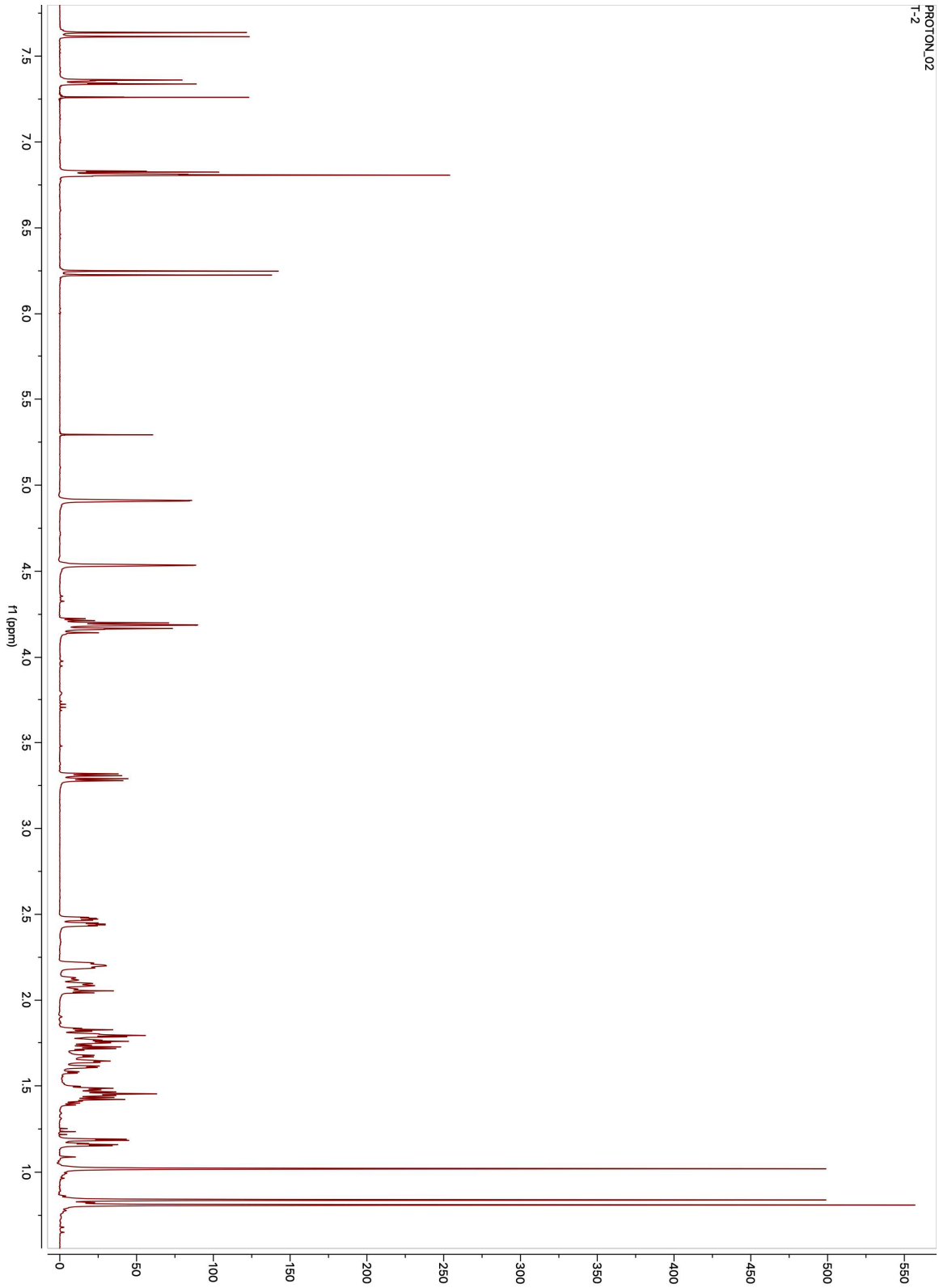


Fig. S13 ^{1}H NMR spectrum of Colladonin (**5**)

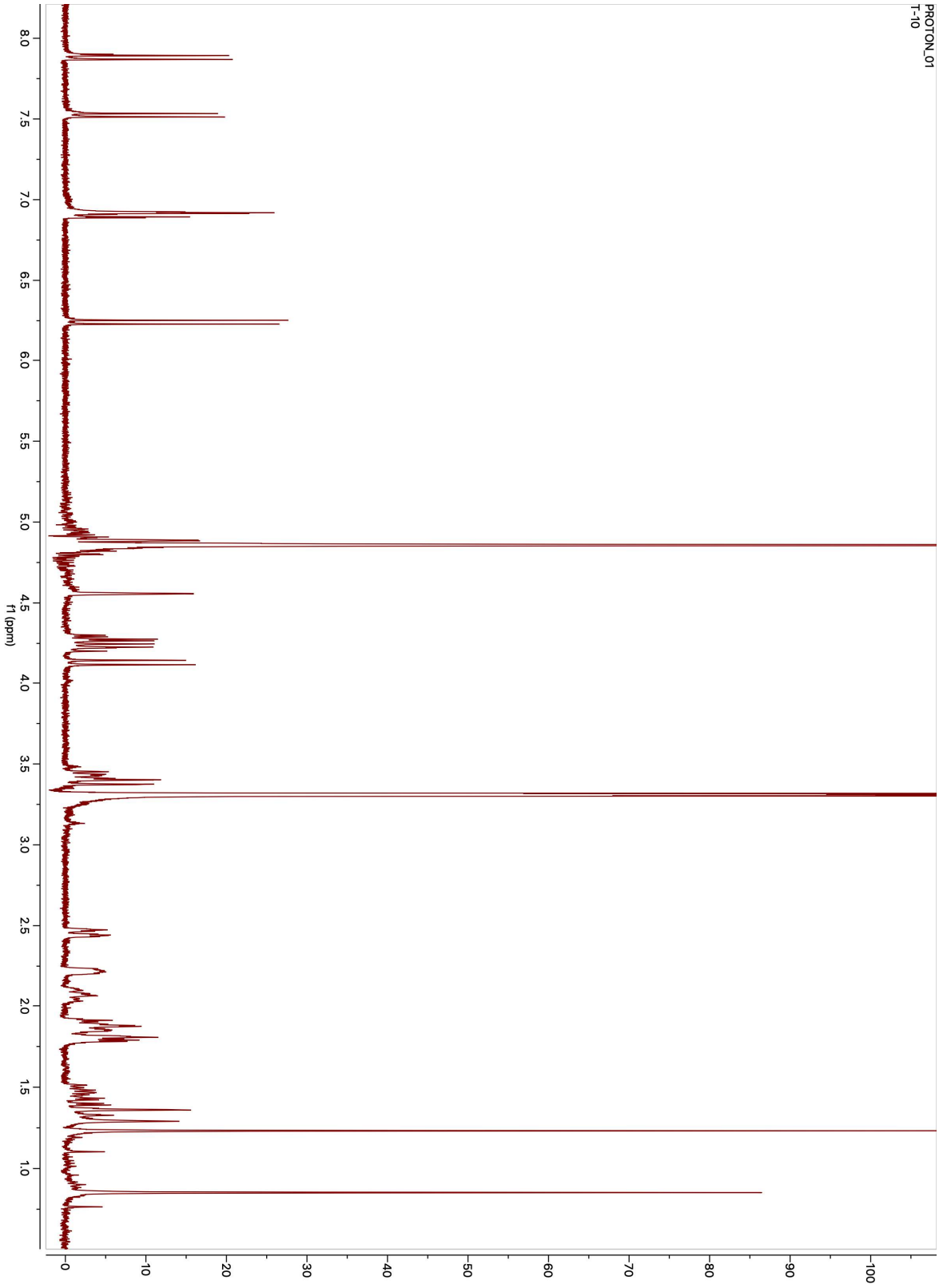


Fig. S14 ^{1}H NMR spectrum of 14'-Hydroxycolladonin (**6**)

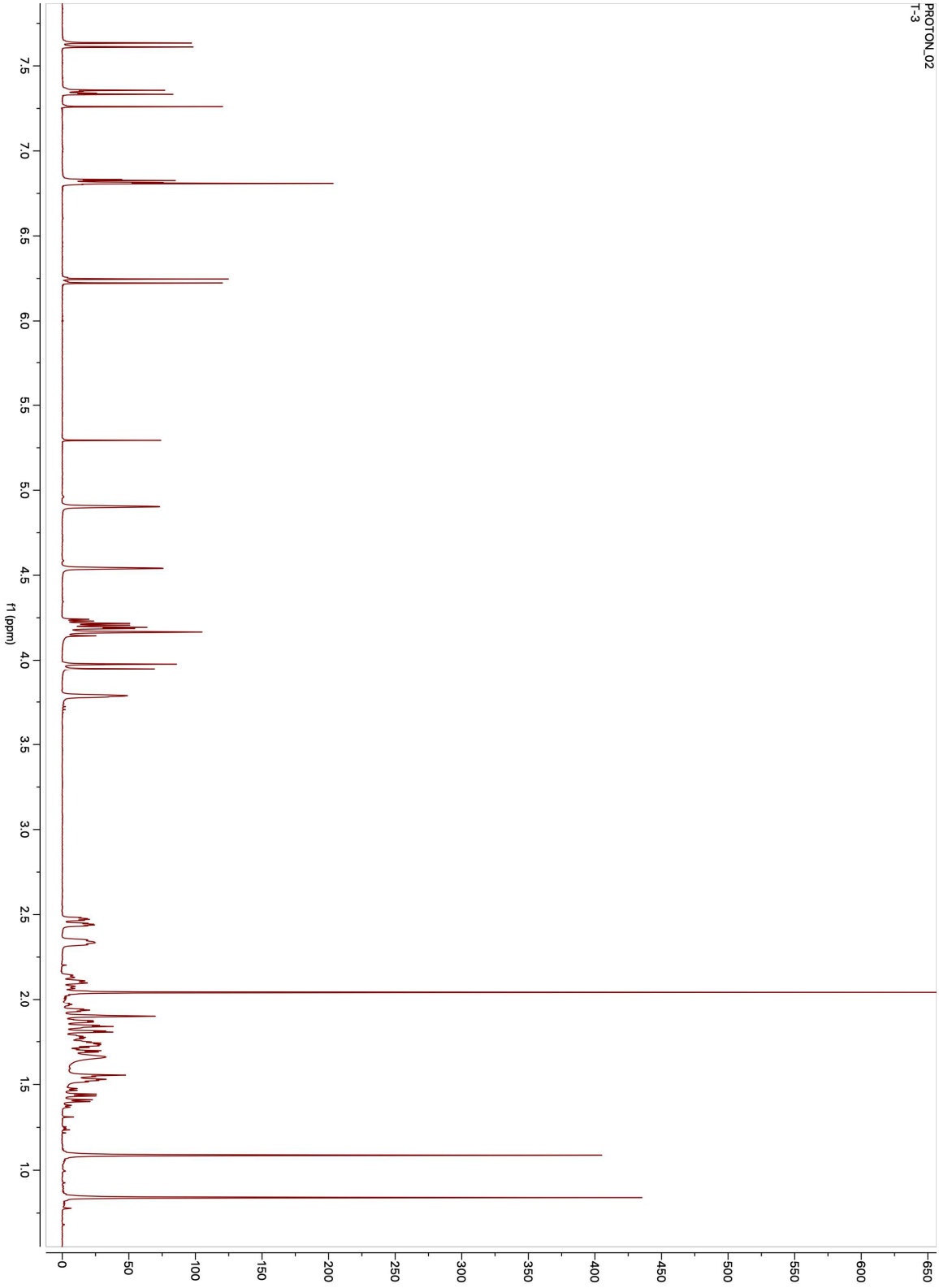


Fig. S15 ^{1}H NMR spectrum of 14'-Acetoxybadrakemin (**7**)