

Electronic Supplementary Information (ESI†)

Discovery and activity profiling of thailandepsins A through F, potent histone deacetylase inhibitors, from *Burkholderia thailandensis* E264†

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Table S1 NMR spectroscopic data of thailandepsin C (**3**)

	position	δ_C , type	δ_H (J in Hz)	HMBC
Met	1	170.5, C=O		2, 3, NH'
	2	58.0, CH	4.43, m	3, 4, NH
	3	28.2, CH ₂	2.36, m	2, 4, NH
			2.18, m	
	4	31.8, CH ₂	2.87, m	2, 3, 5
			2.72, m	
5	16.0, CH ₃	2.26, s	3, 4	
	NH		7.73, d (3.2)	
Cys	1'	169.4, C=O		2'', 4'', NH''
	2'	55.2, CH	4.97, m	
	3'	41.6, CH ₂	3.33, m	
			3.25, m	
	NH'		6.83, d (9.5)	
Ahhx ^a	1''	172.4, C=O		2''
	2''	40.1, CH ₂	2.75, m	
	3''	69.8, CH	4.63, br s	2'', 4'', 5'', HN''
	4''	64.2, CH	2.80, m	2'', 5'', 6'', 7''
	5''	30.1, CH	2.48, m	4'', 6'', 7''
	6''	21.1, CH ₃	1.09, d (6.8)	4'', 5'', 7''
	7''	20.1, CH ₃	0.99, d (6.8)	4'', 5'', 6''
		NH''		7.49, d (7.0)
	OH''			
acyl	1'''	171.3, C=O		2, 4, 2''', NH
	2'''	41.4, CH ₂	3.43, m	
	3'''	71.2, CH	5.56, br s	2''', 4''', 6'''
	4'''	129.6, CH	5.76, d (15.4)	2''', 6'''
	5'''	133.8, CH	6.39, m	
	6'''	33.8, CH ₂	2.76, m	4'''
			2.47, m	
	7'''	41.8, CH ₂	2.79, m	
2.65, m				

^aAhhx: 4-amino-3-hydroxy-5-methylhexanoic acid.

Fig. S1 Analytical HPLC traces of purified thailandepsins A through F (1–6), indicating an estimated purity between 90% to 96% for individual compound

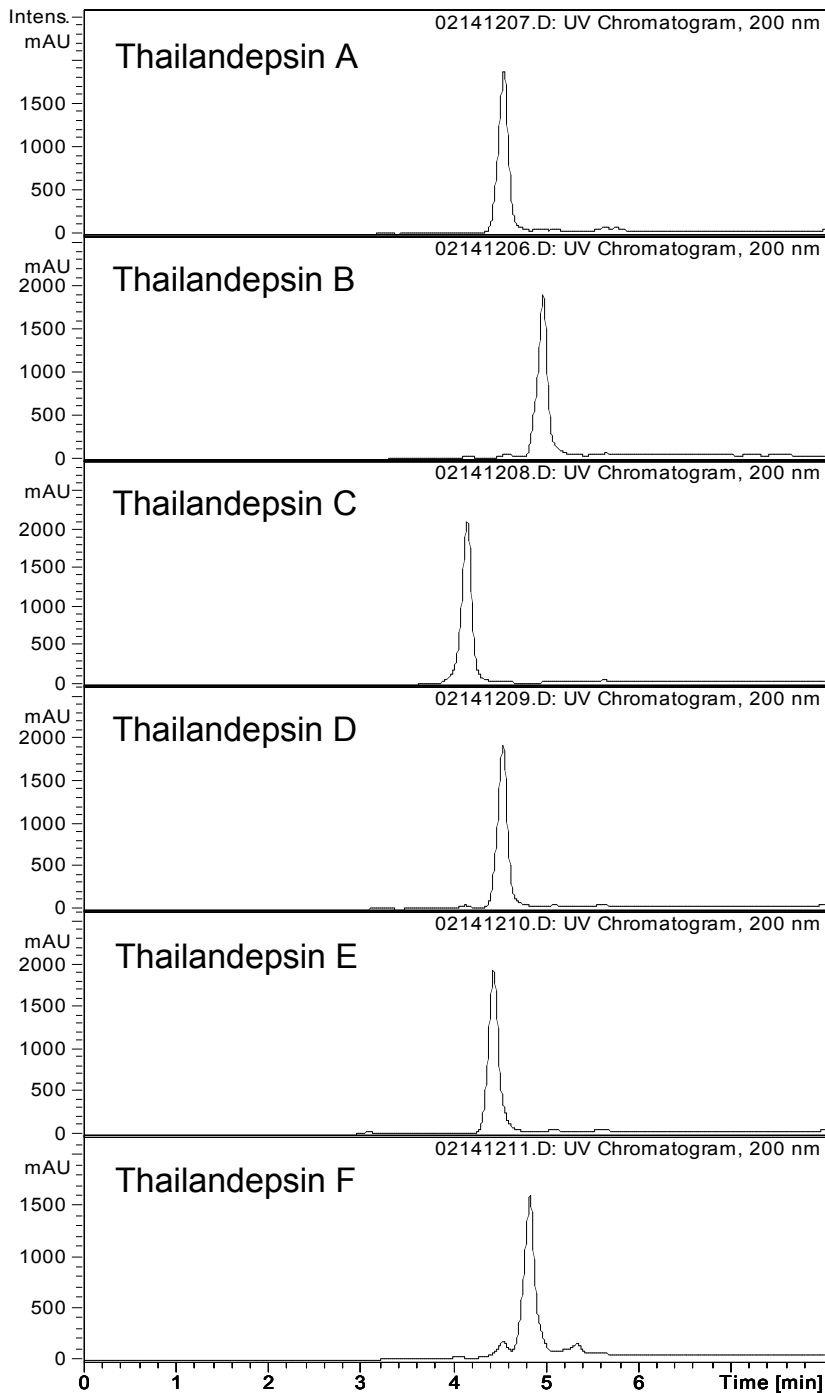


Fig. S2 ^1H NMR (300 MHz, CDCl_3) spectrum of thailandepsin C (**3**)

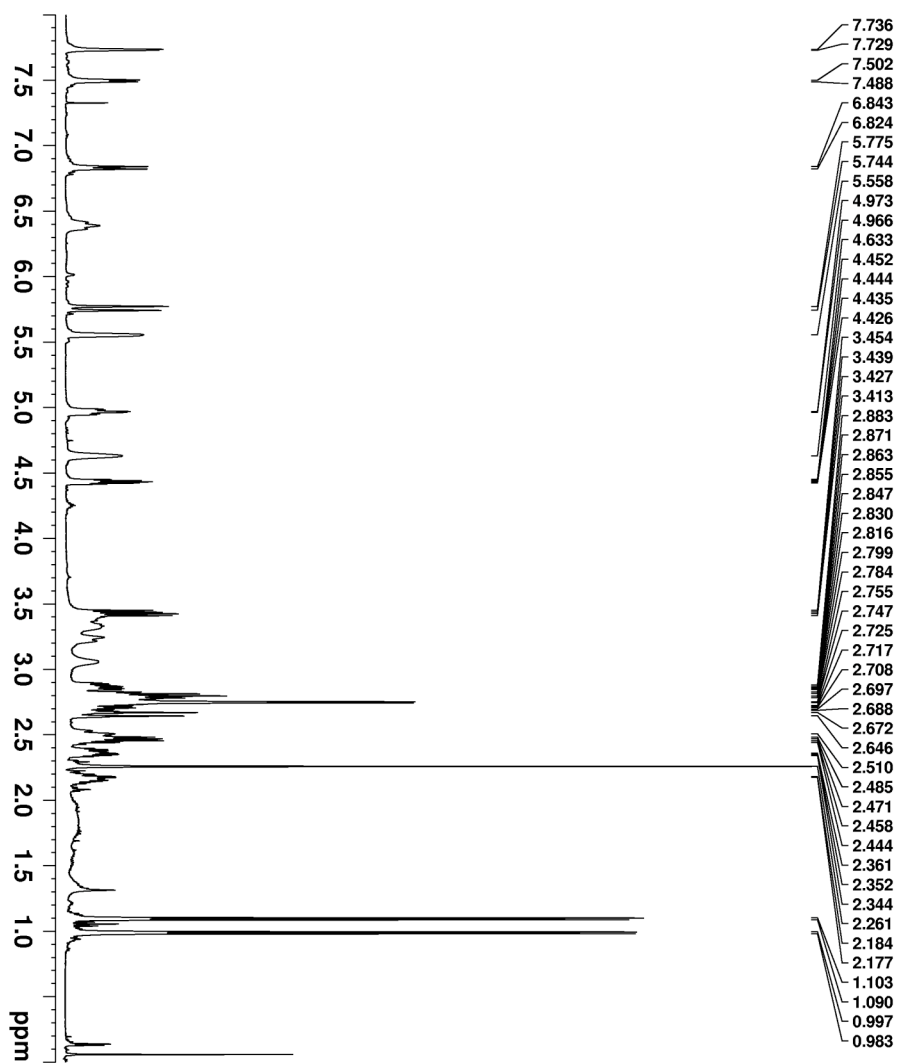


Fig. S3 ^{13}C NMR (300 MHz, CDCl_3) spectrum of thailandepsin C (**3**)

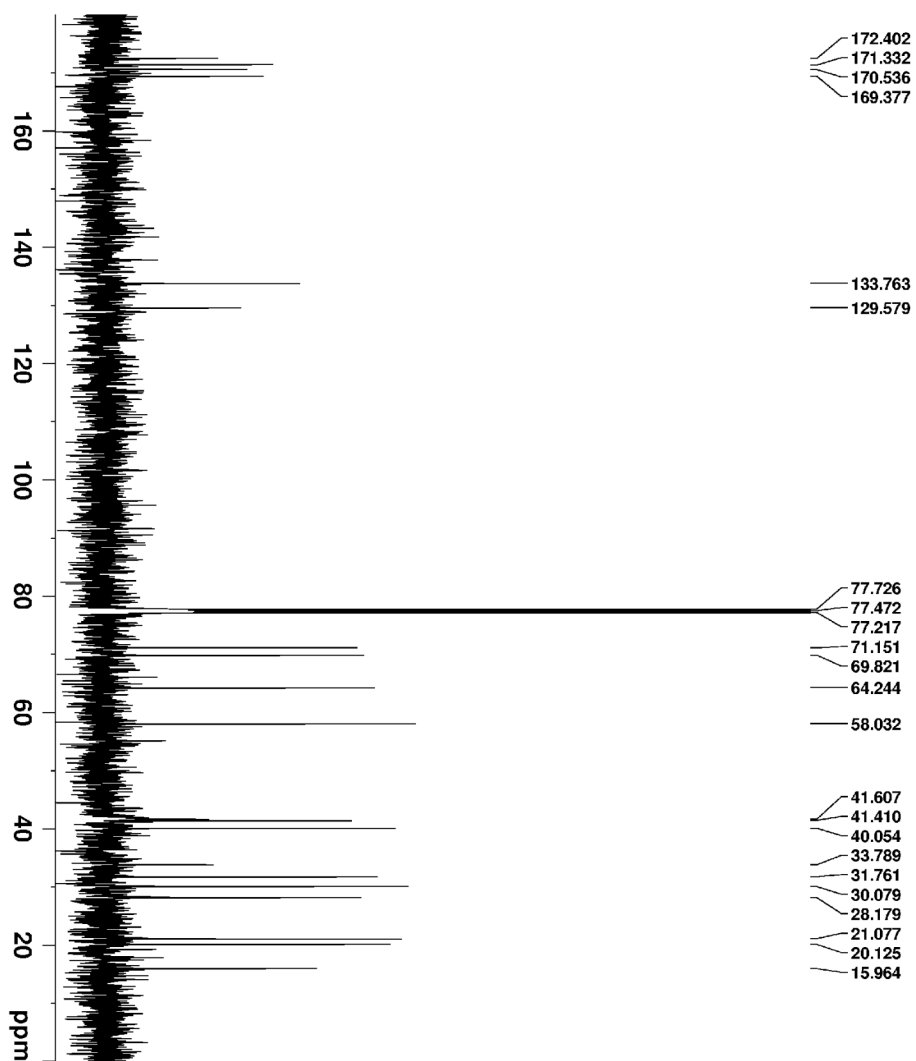


Fig. S4 Edit_HSQC spectrum of thailandepsin C (3)

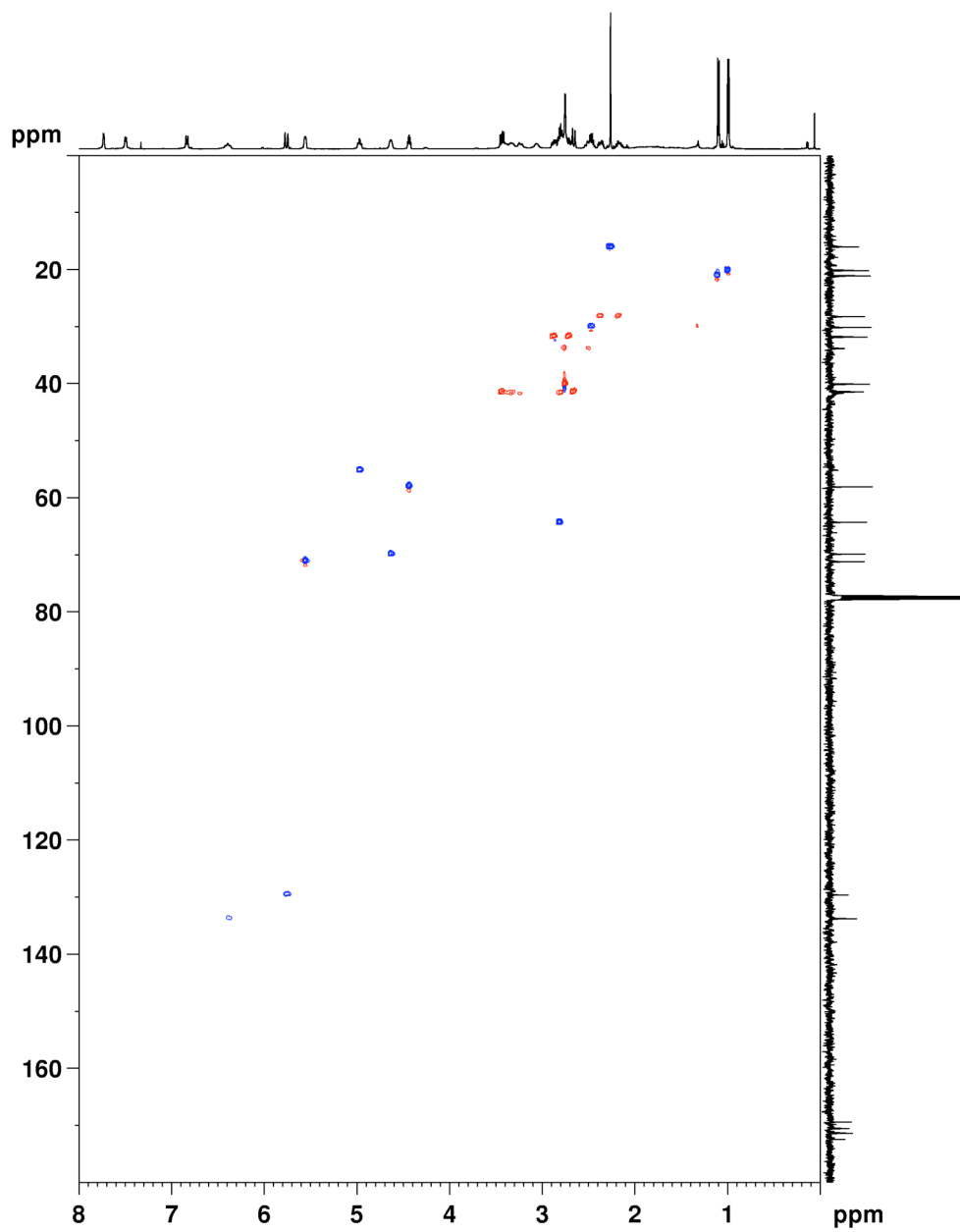


Fig. S5 ^1H - ^1H COSY spectrum of thailandepsin C (**3**)

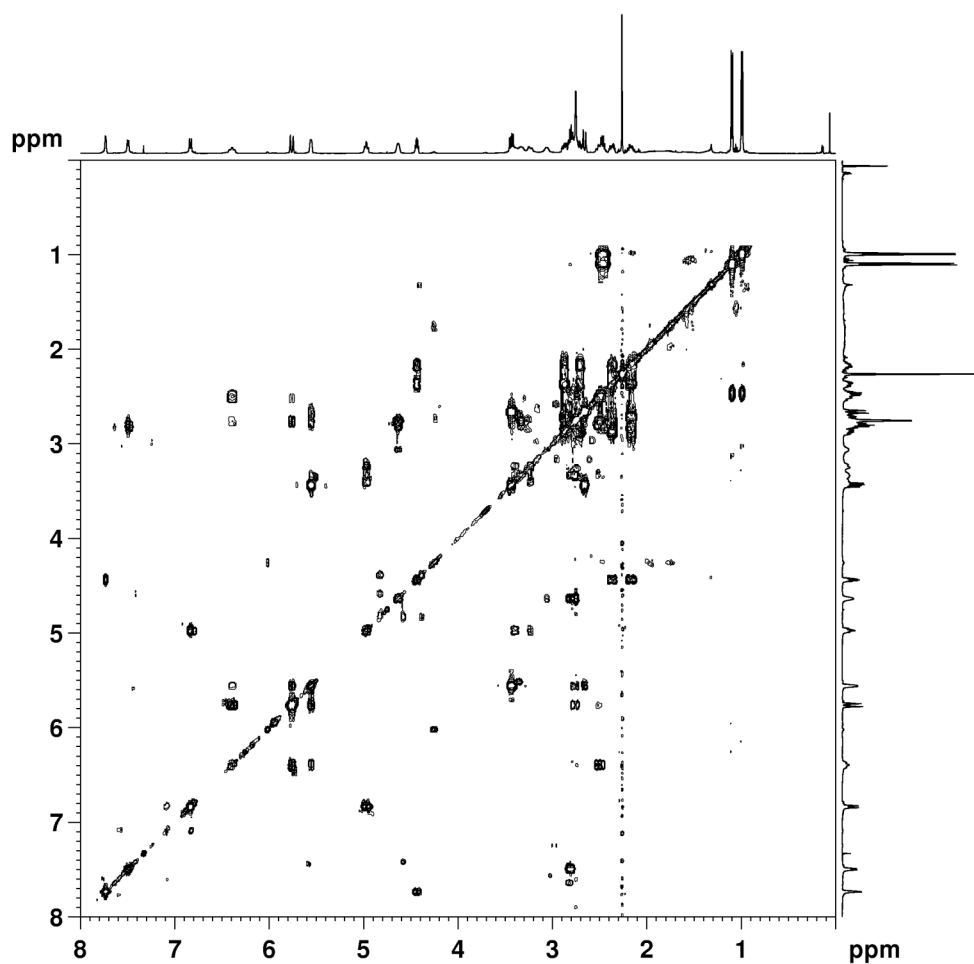


Fig. S6 HMBC spectrum of thailandepsin C (**3**)

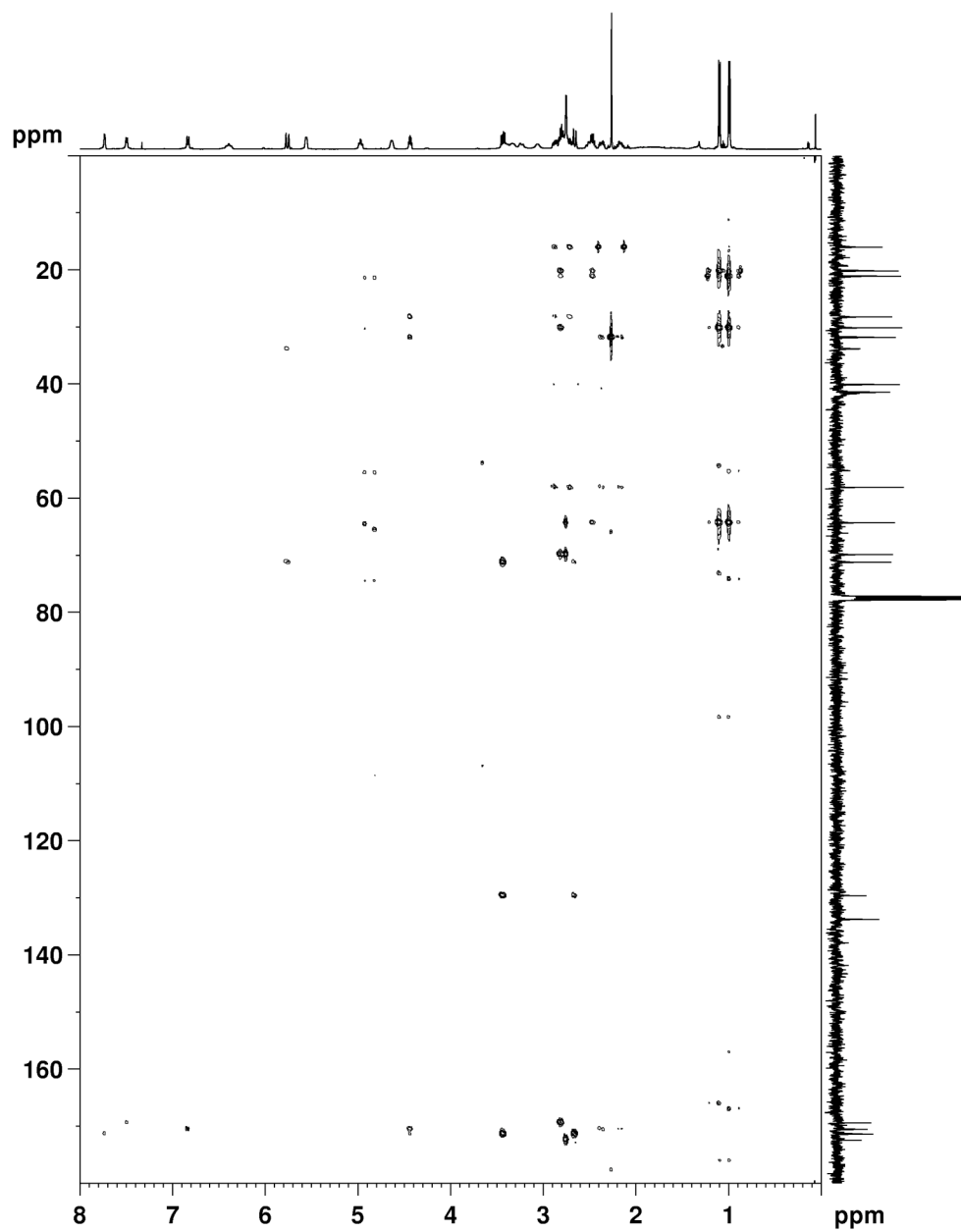


Fig. S7 HR-TOF-MS spectrum of thailandepsin D (4)

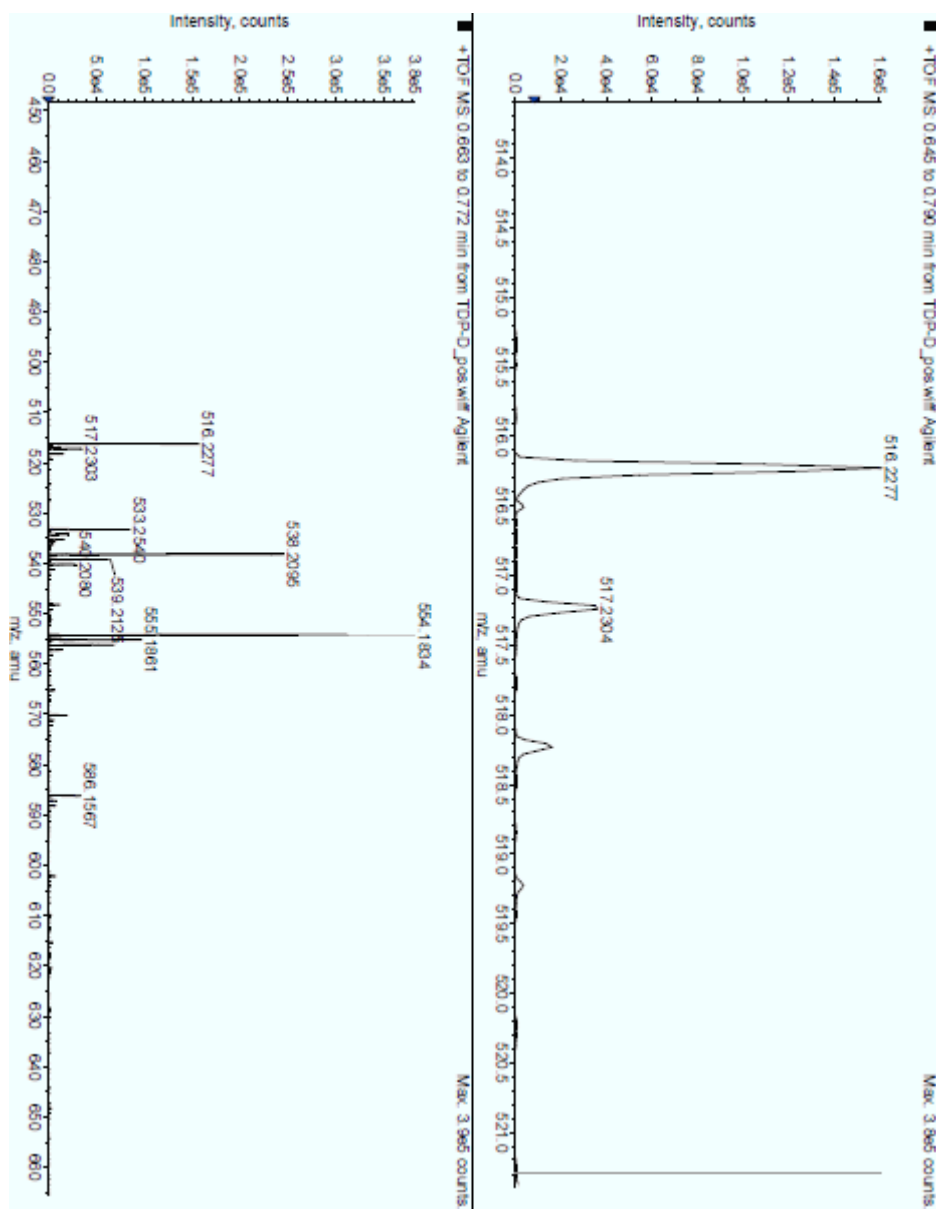


Fig. S8 ^1H NMR (300 MHz, CDCl_3) spectrum of thailandepsin D (4)

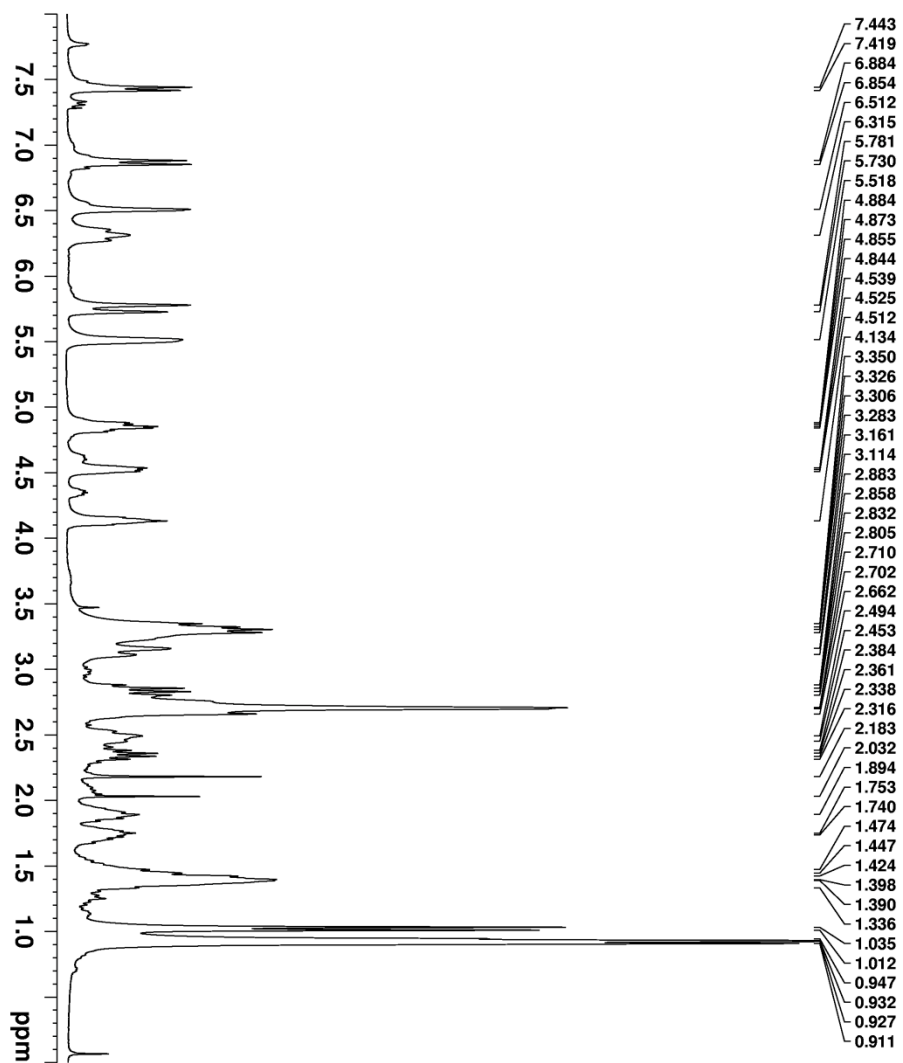


Fig. S9 ^{13}C NMR (300 MHz, CDCl_3) spectrum of thailandepsin D (4)

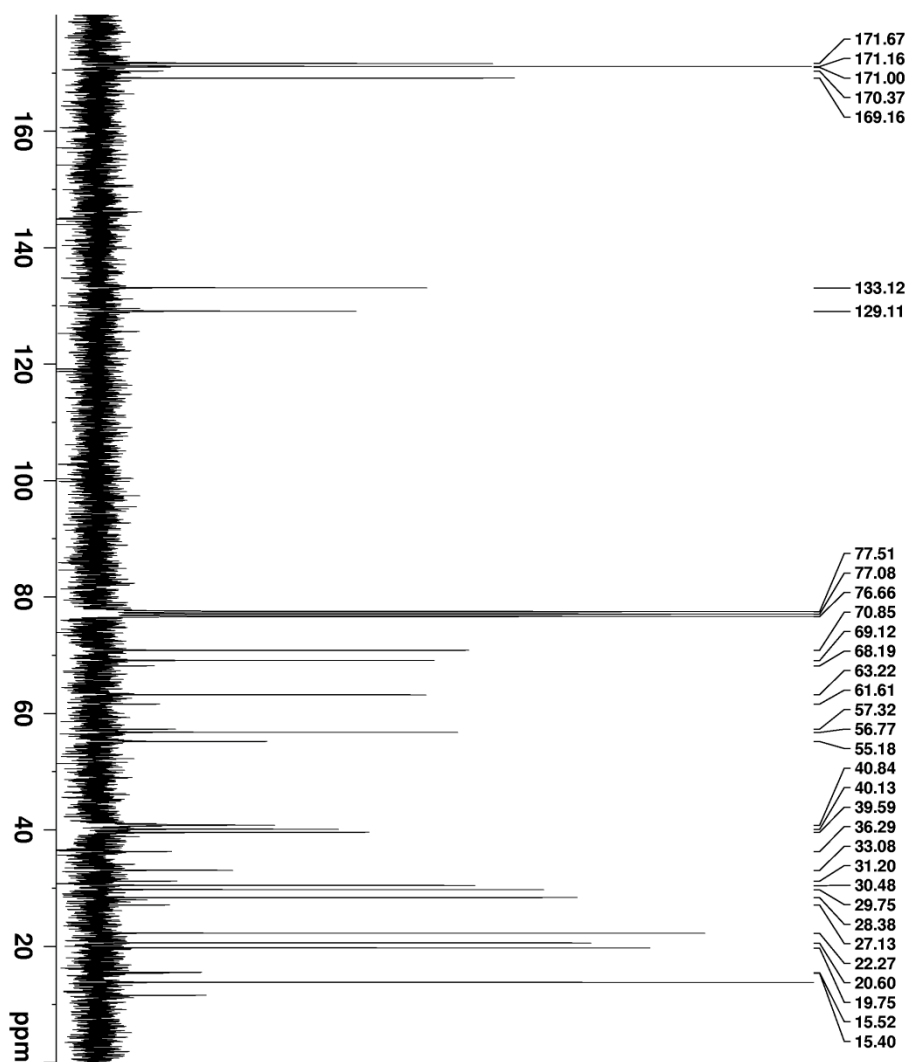


Fig. S10 DEPT (300 MHz, CDCl₃) spectrum of thailandepsin D (4)

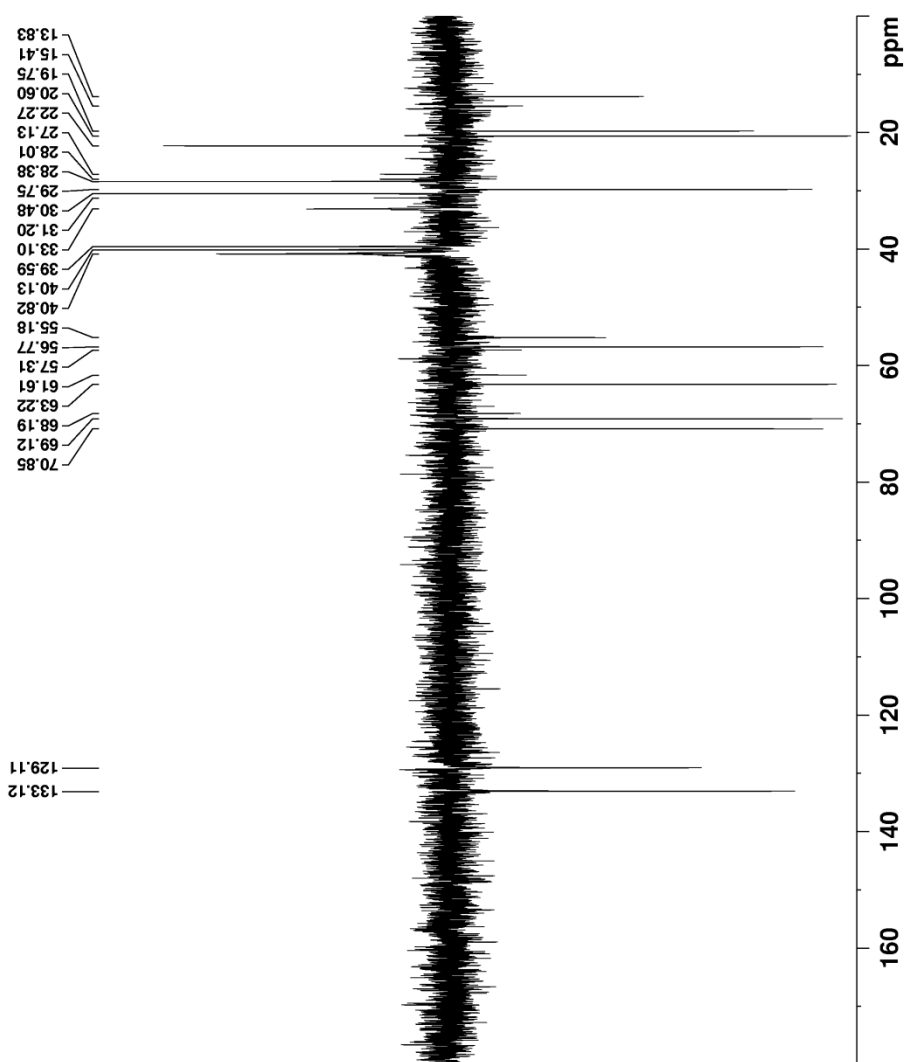


Fig. S11 Edit_HSQC spectrum of thailandepsin D (4)

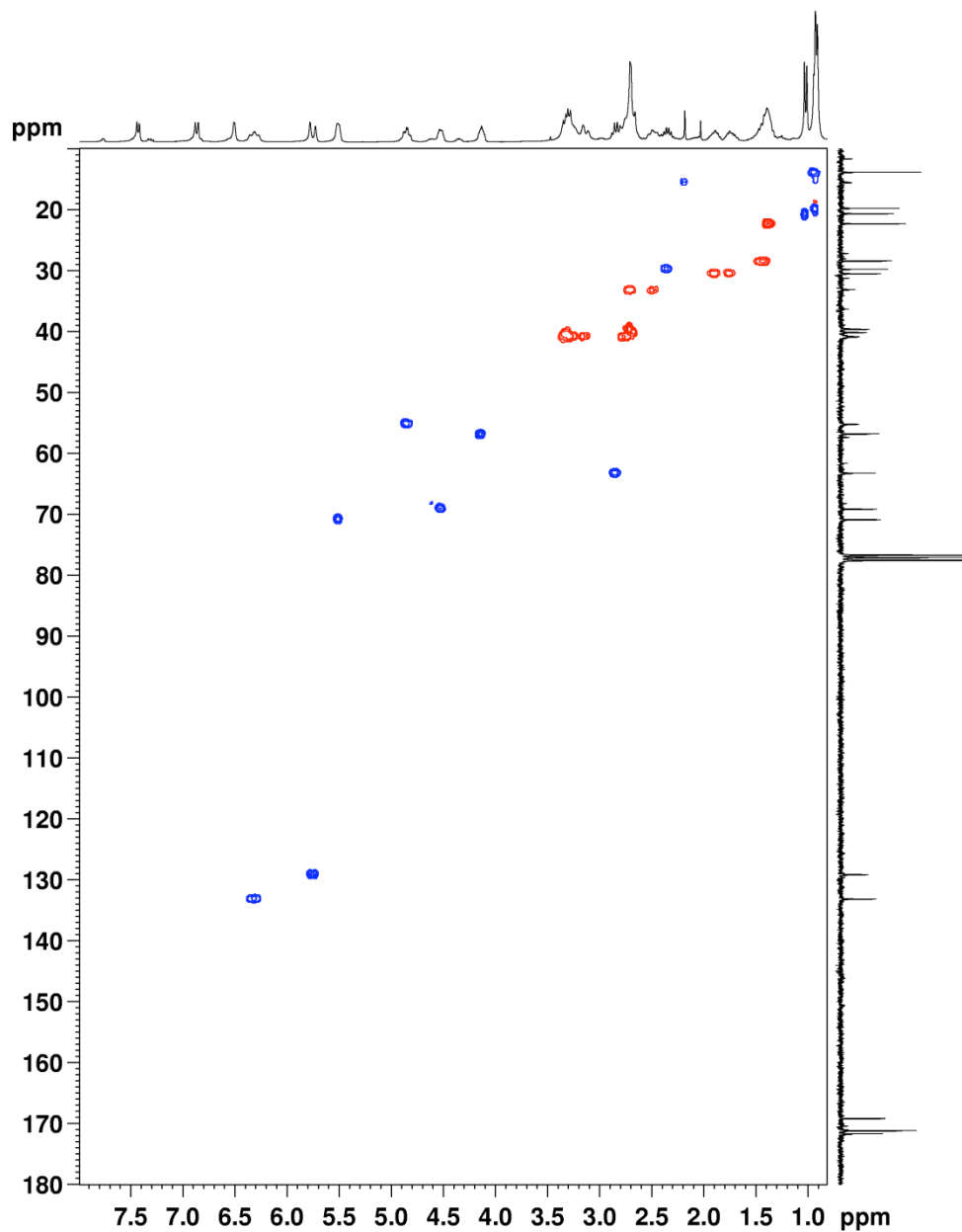


Fig. S12 ^1H - ^1H COSY spectrum of thailandepsin D (**4**)

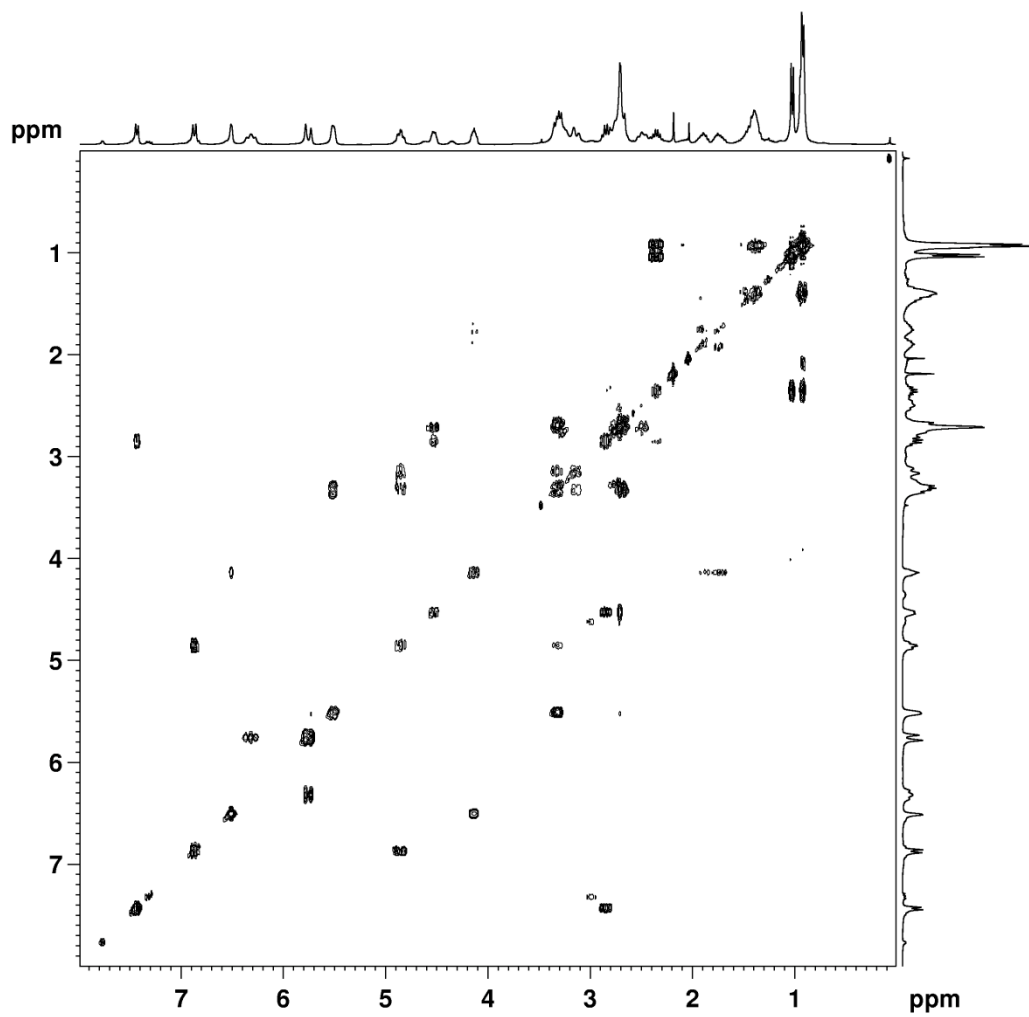


Fig. S13 HMBC spectrum of thailandepsin D (4)

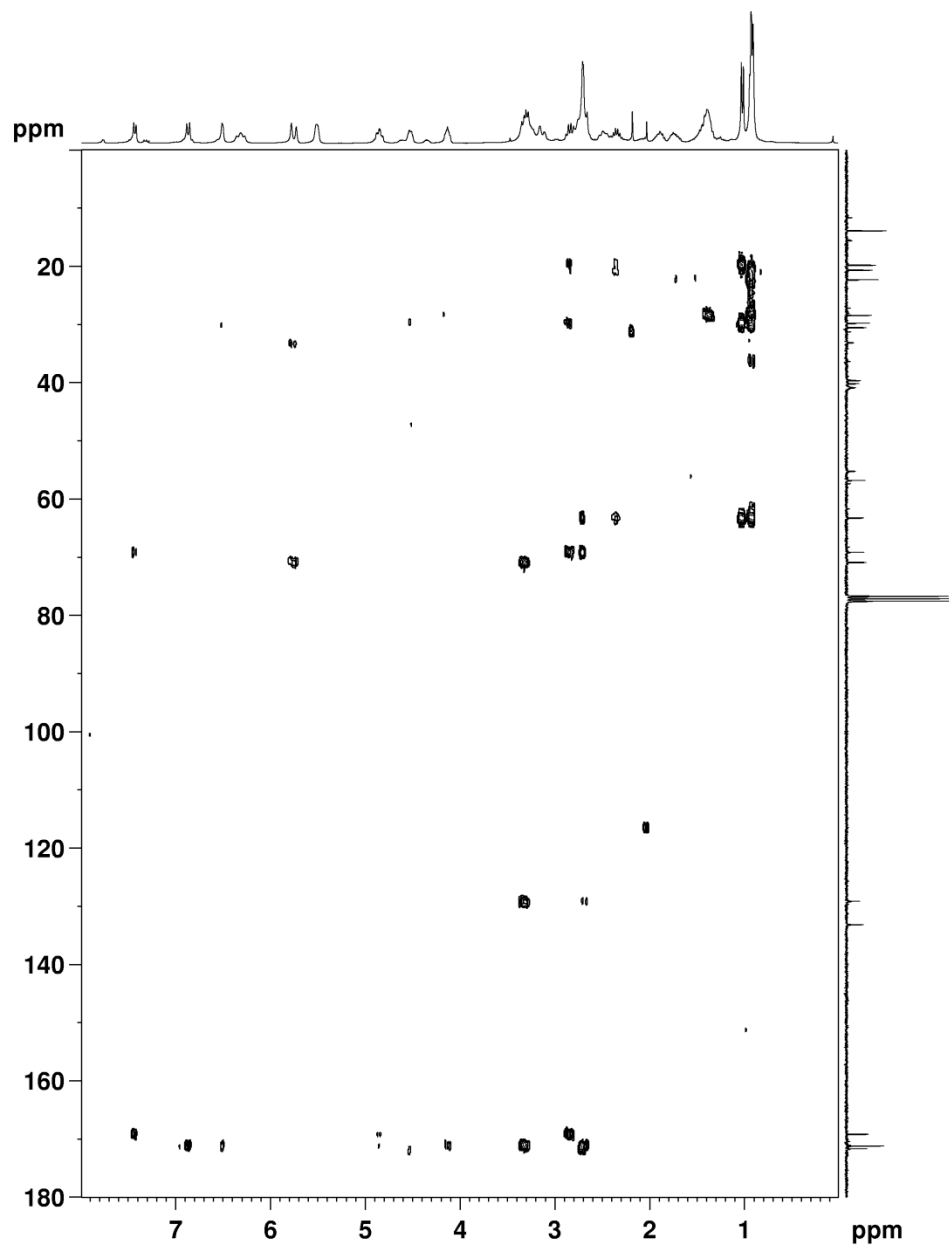


Fig. S14 HR-TOF-MS spectrum of thailandepsin E (5)

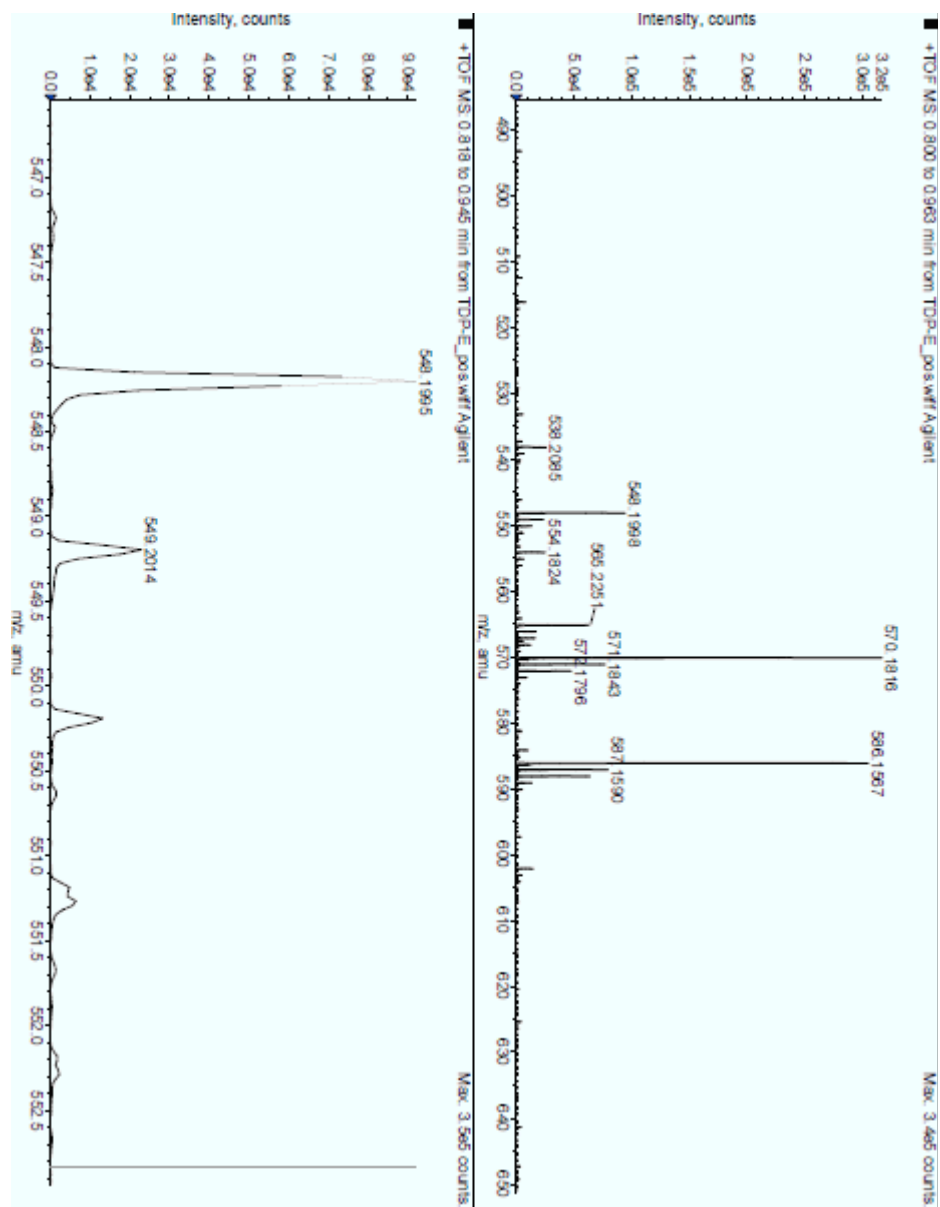


Fig. S15 ^1H NMR (300 MHz, CDCl_3) spectrum of thailandepsin E (**5**)

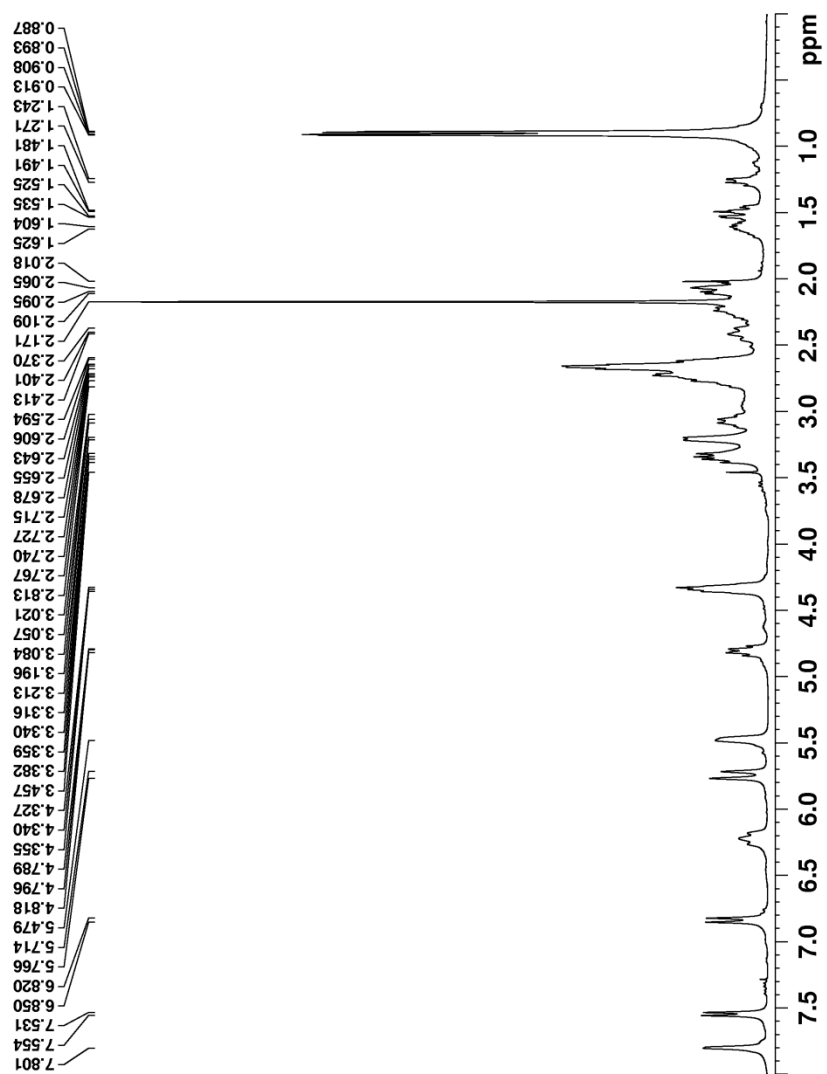


Fig. S16 ^{13}C NMR (300 MHz, CDCl_3) spectrum of thailandepsin E (5)

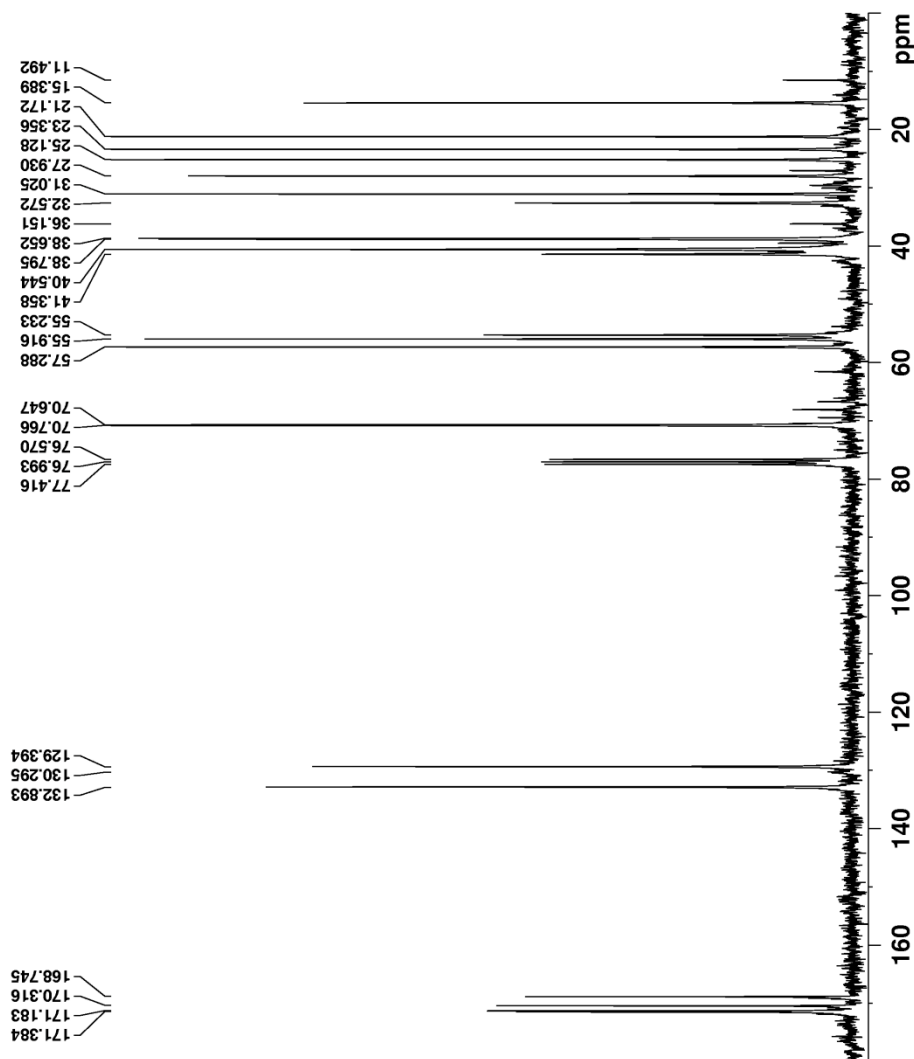


Fig. S17 Edit_HSQC spectrum of thailandepsin E (5)

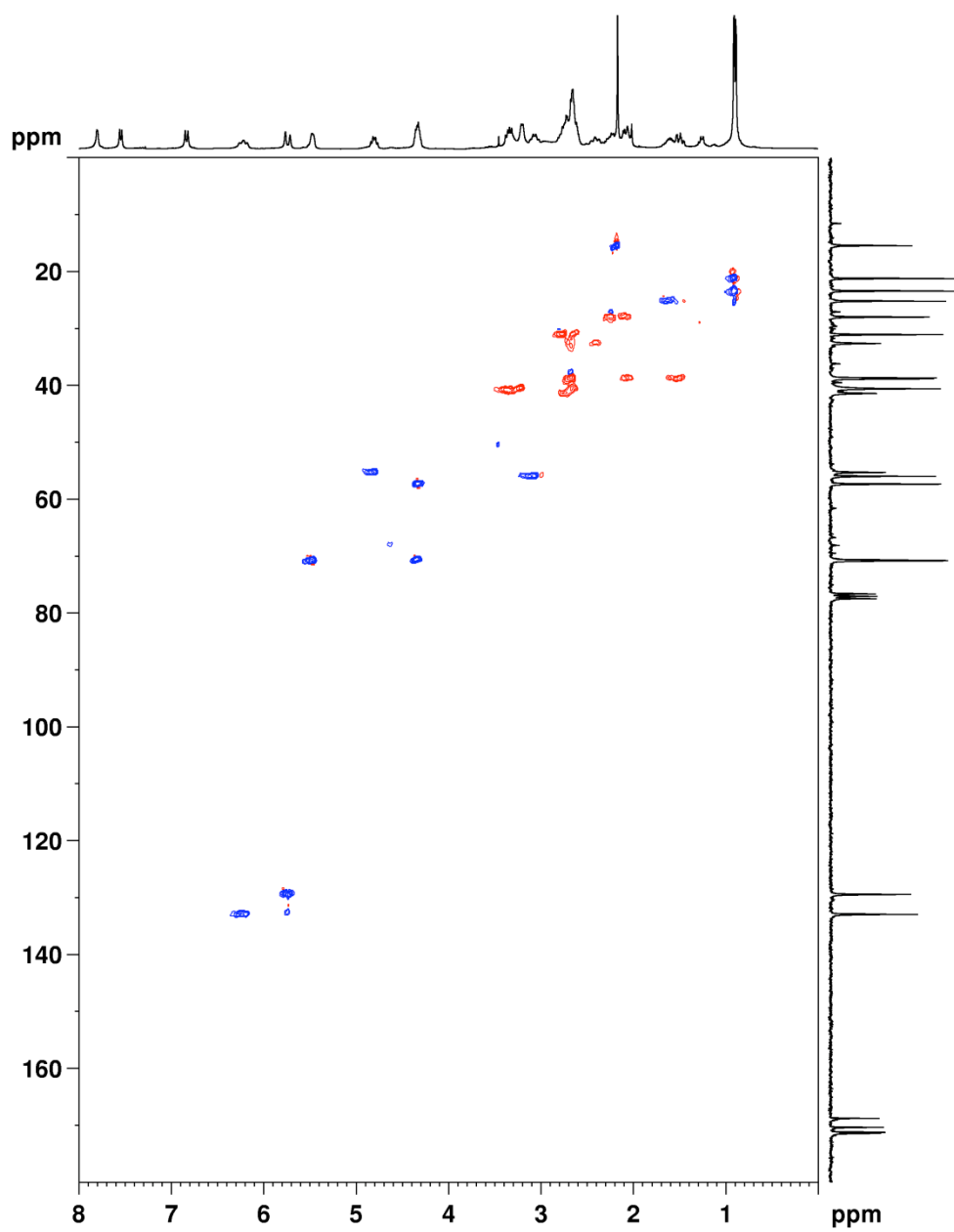


Fig. S18 ^1H - ^1H COSY spectrum of thailandepsin E (**5**)

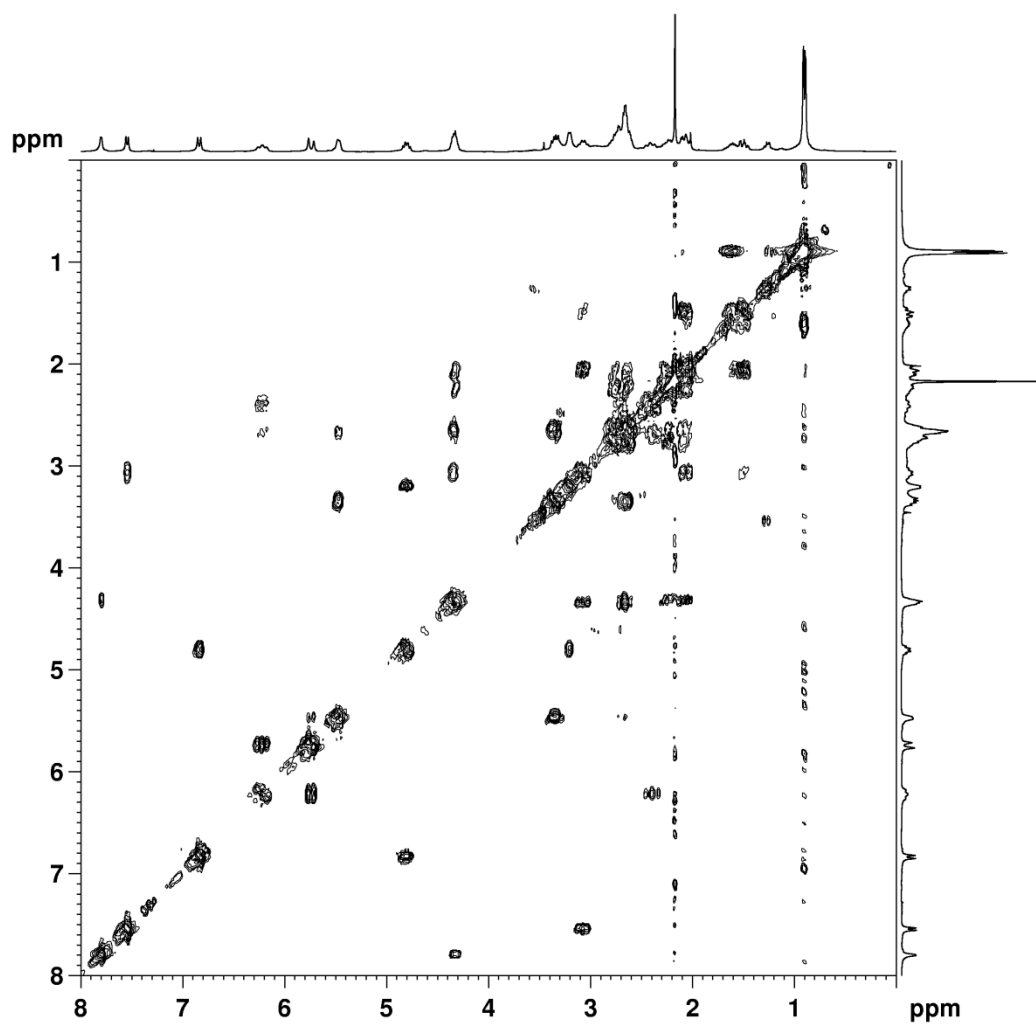


Fig. S19 HMBC spectrum of thailandepsin E (5)

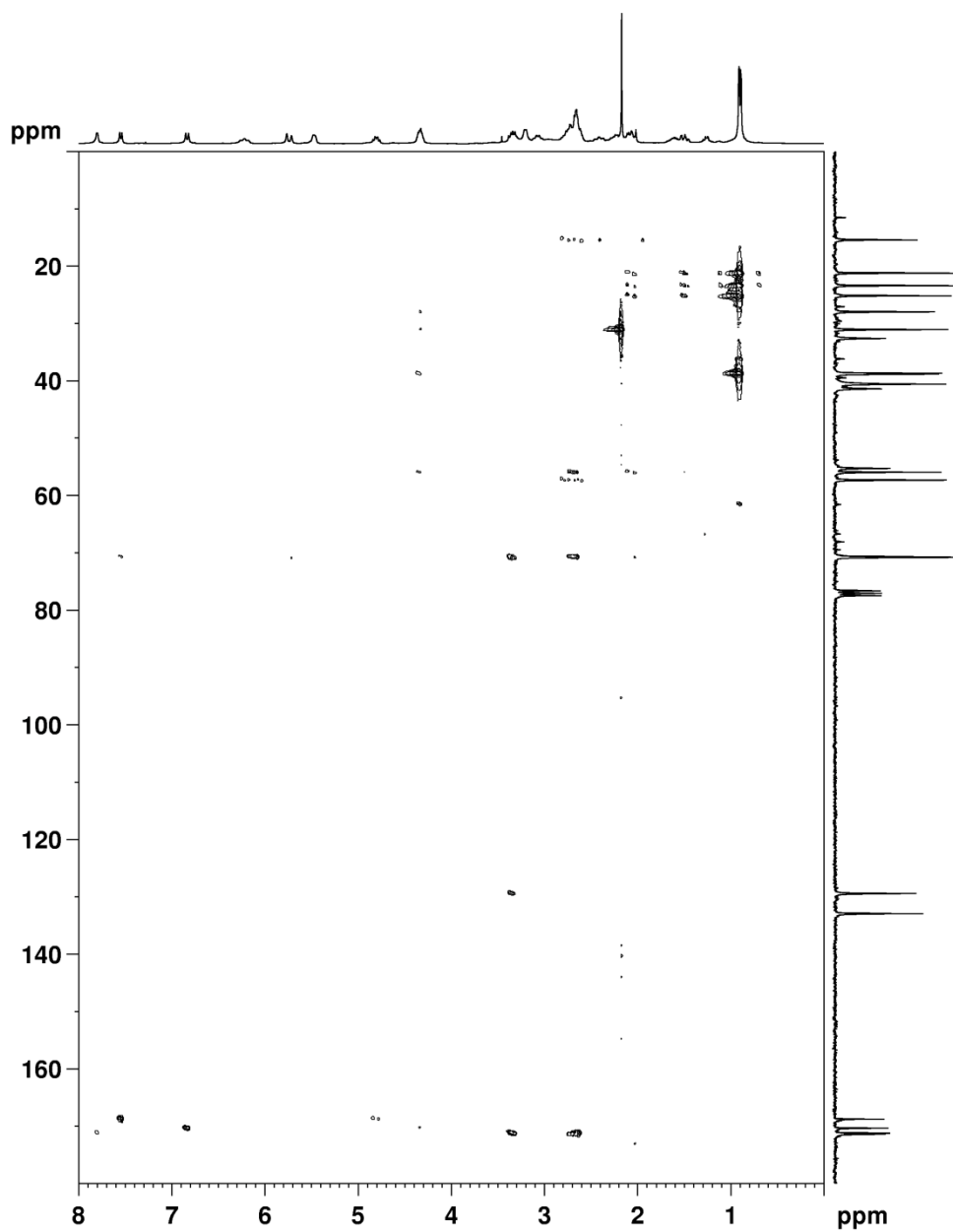


Fig. S20 HR-TOF-MS spectrum of thailandepsin F (6)

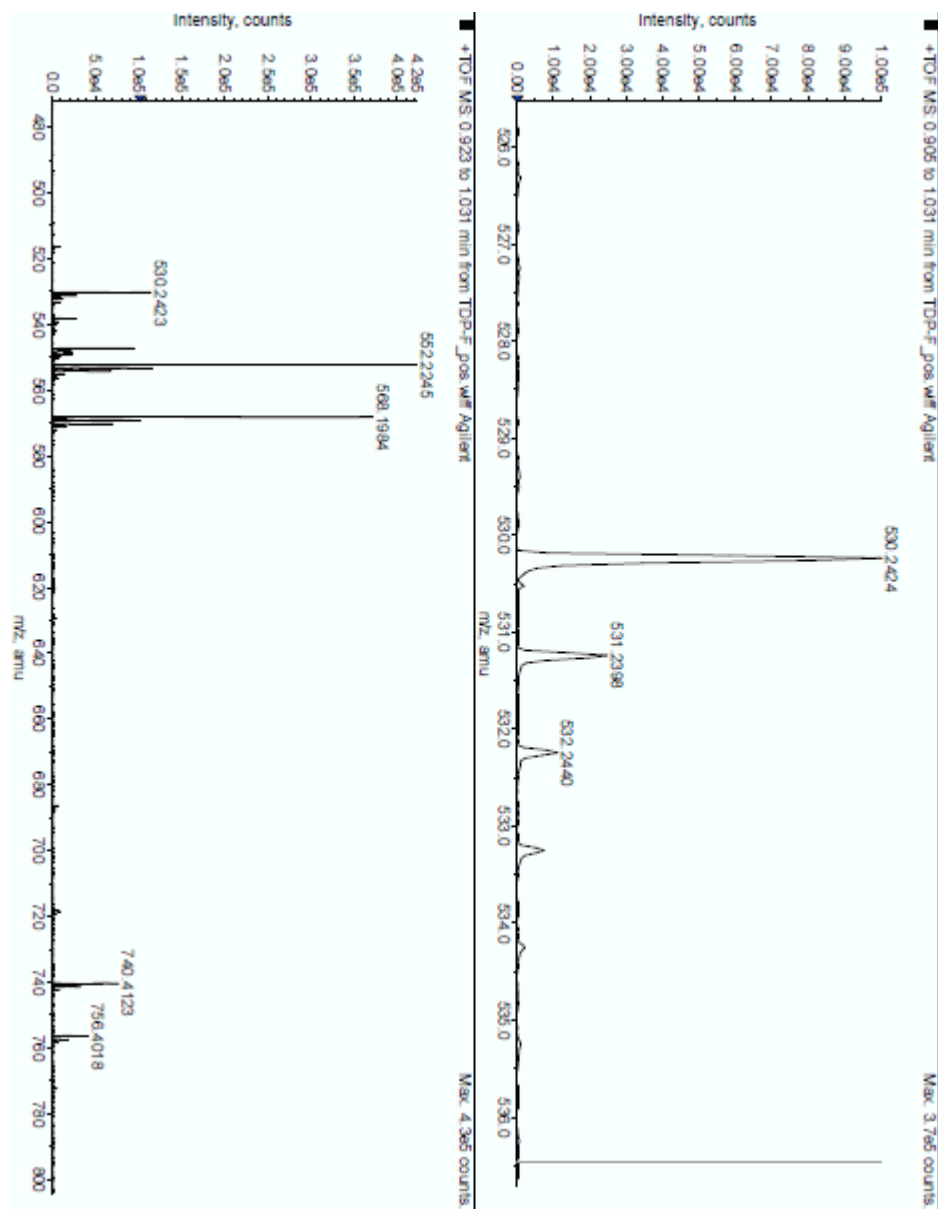


Fig. S21 ^1H NMR (300 MHz, CDCl_3) spectrum of thailandepsin F (**6**)

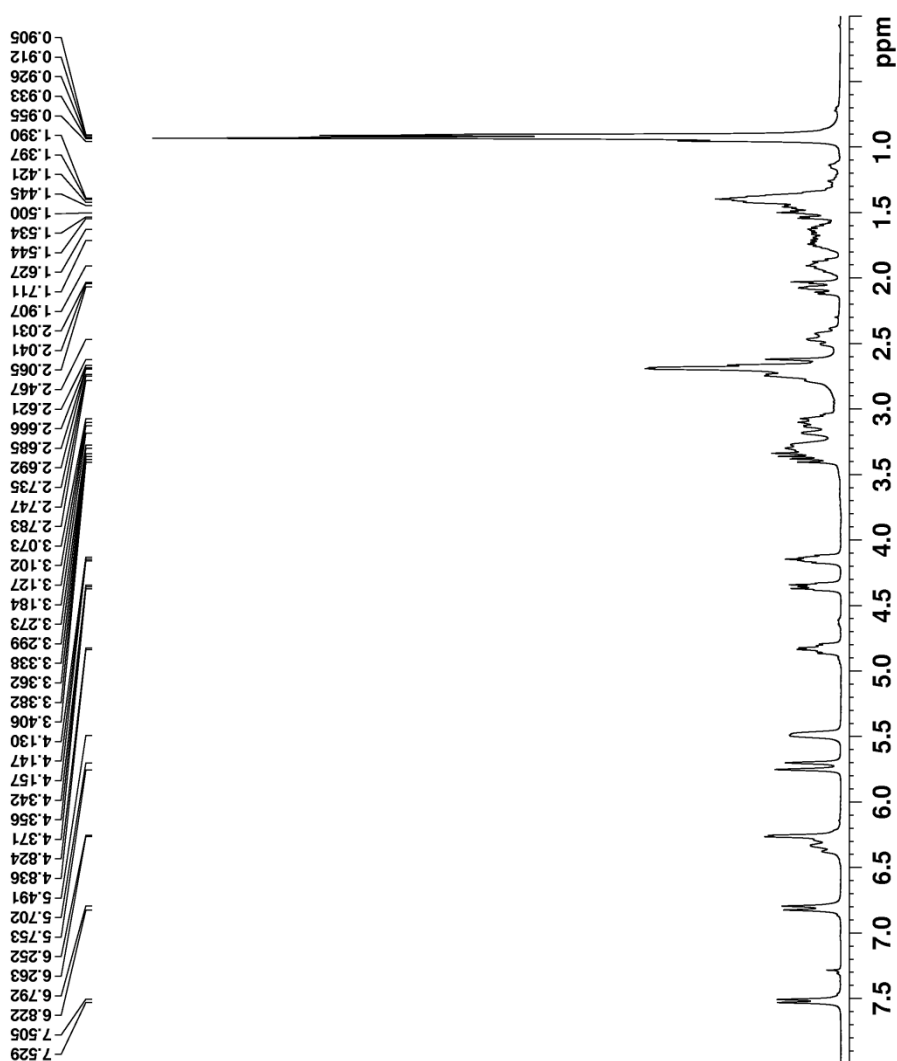


Fig. S22 ^{13}C NMR (300 MHz, CDCl_3) spectrum of thailandepsin F (6)

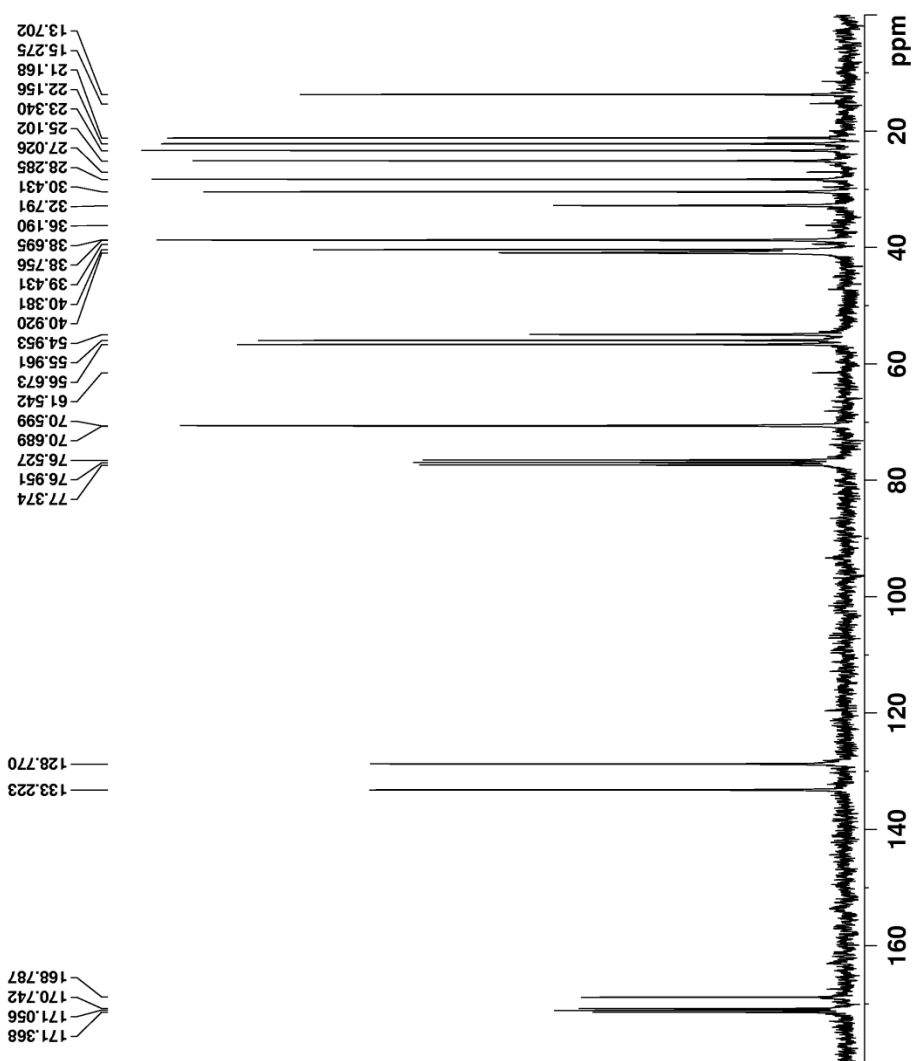


Fig. S23 Edit_HSQC spectrum of thailandepsin F (6)

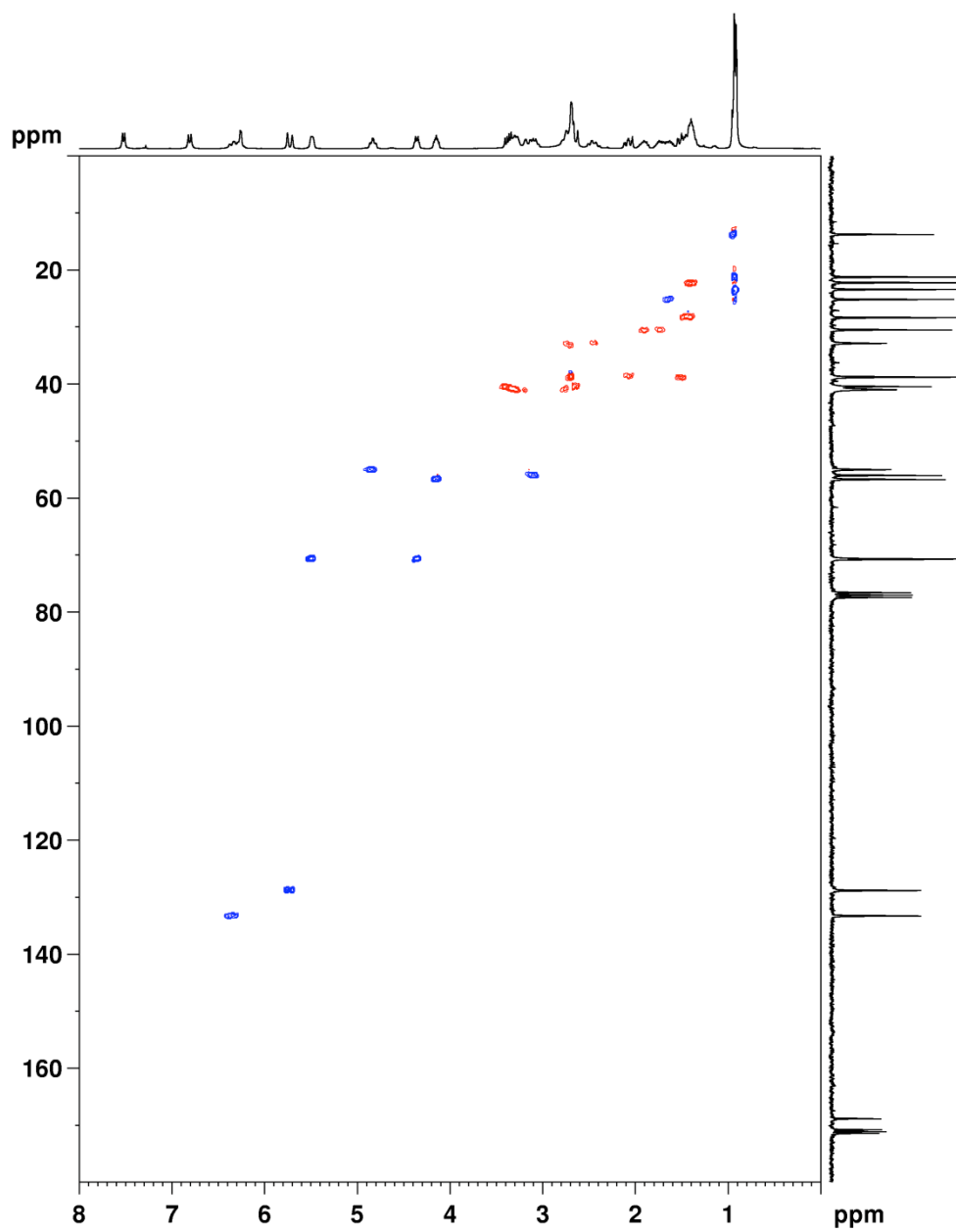


Fig. S24 ^1H - ^1H COSY spectrum of thailandepsin F (6)

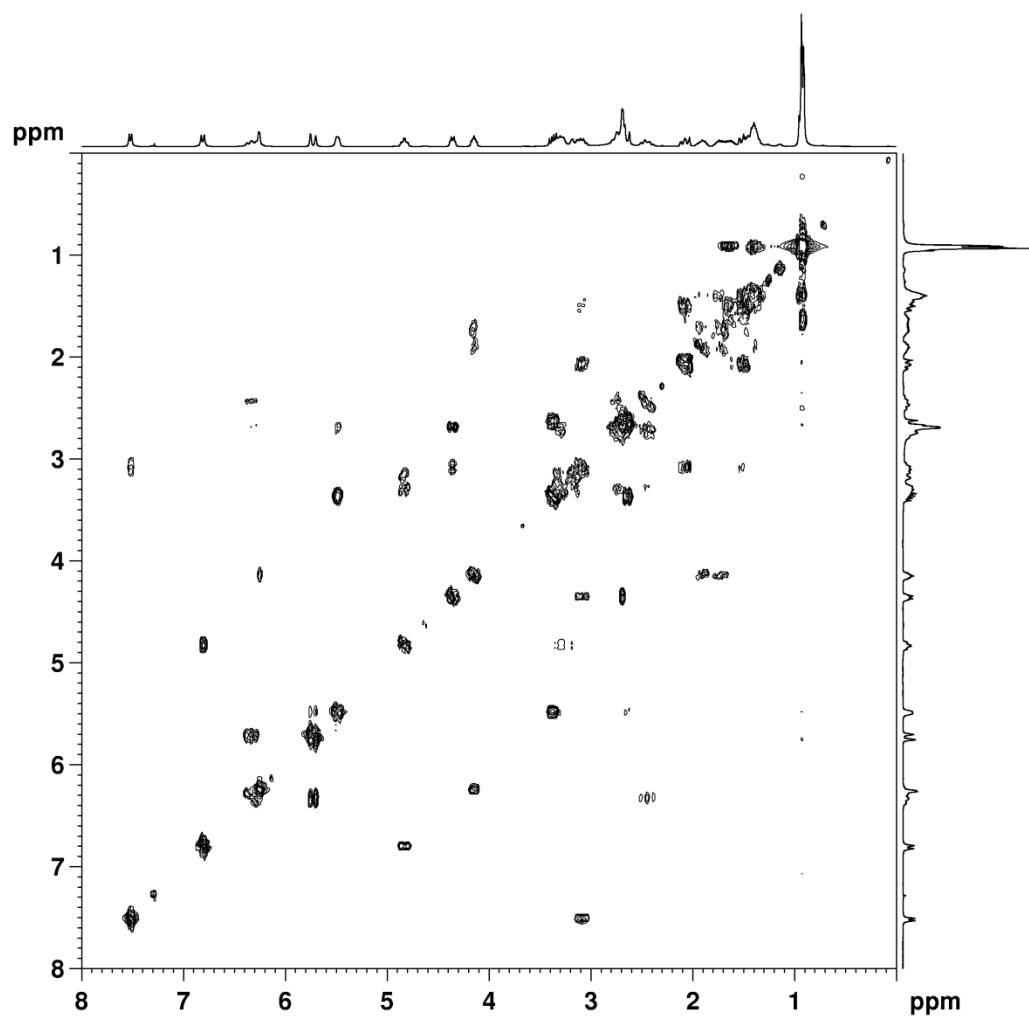


Fig. S25 HMBC spectrum of thailandepsin F (6)

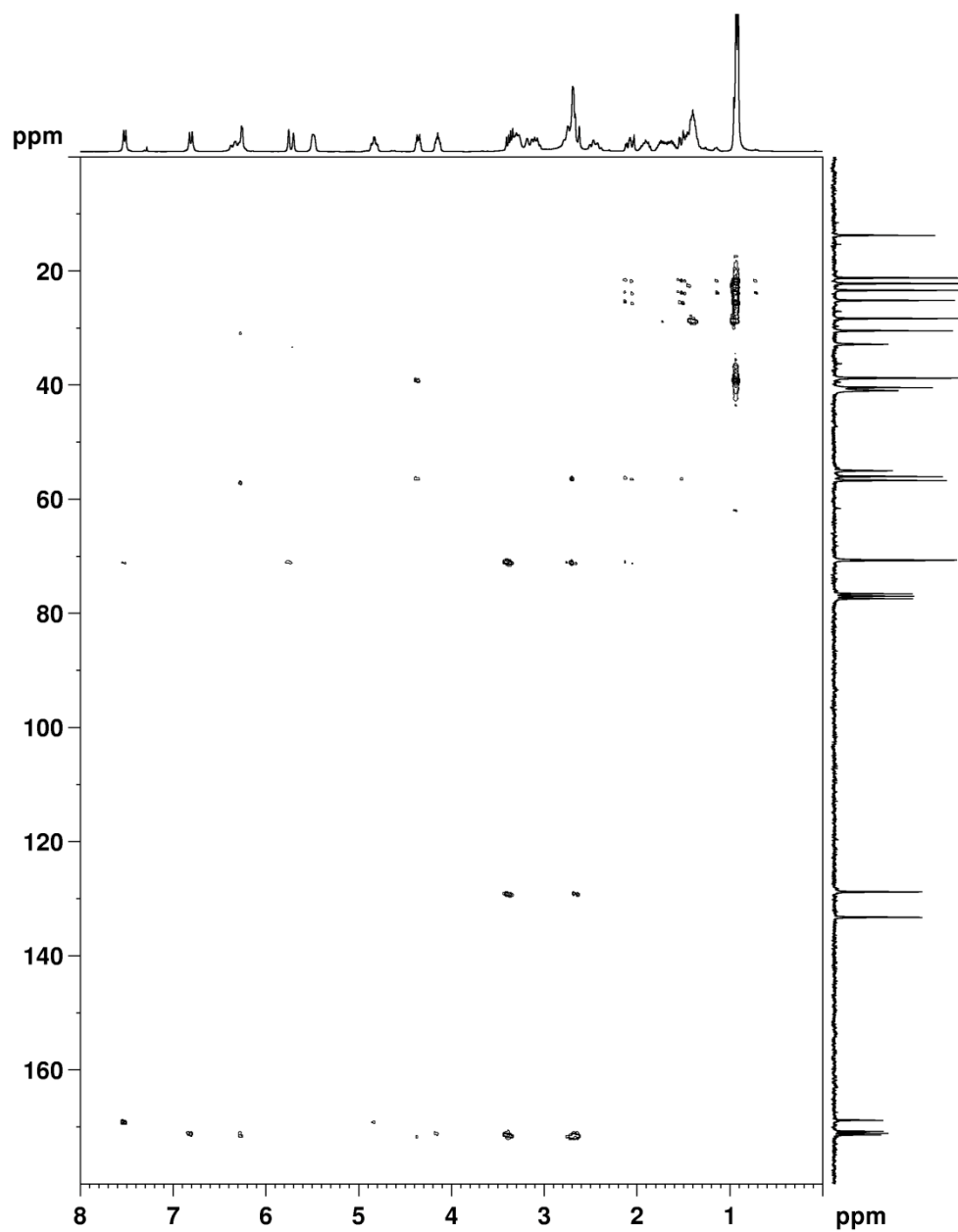
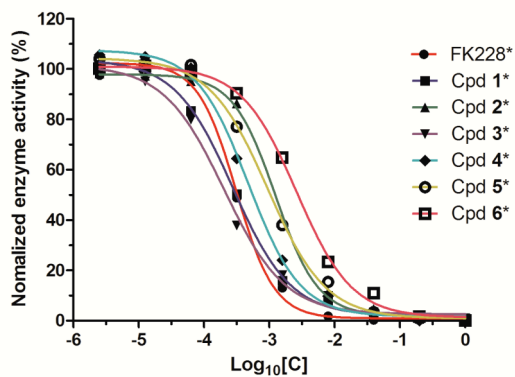
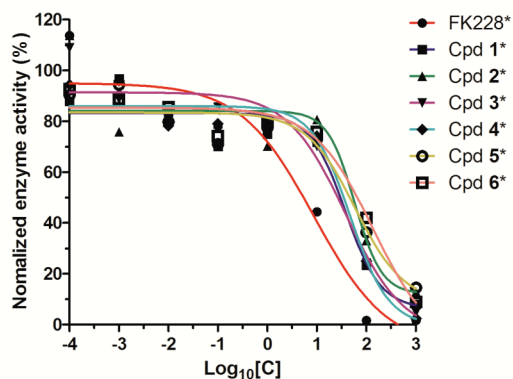


Fig. S26 Enzyme inhibitory assays. (a) Dose-response curves of each compound vs. HDAC1; (b) Dose-response curves of each compound vs. HDAC4; (c) Dose-response curves of each compound vs. HDAC6. * indicates compounds in their reduced forms.

a



b



c

