Table S1. ^{1}H and ^{13}C NMR data for compound **1**

Carbon No.	δ_H **1** (600 MHz*)	δ_C **1** (150 MHz)	δ_C (Forgo & Kövér, 2004)
1	1.00 – 1.80	37.27	37.6
2	1.00 – 1.80	31.66	31.9
3	3.53 (m, *J*=4.8 Hz, 1H)	71.80	72.0
4	2.29 (dd, *J* = 6.6, 2.4 Hz, 2H)	42.33	42.5
5	–	140.79	140.8
6	5.36 (dd, *J* = 3.6, 1.2 Hz, 1H)	121.69	121.8
7	2.04 (m, 2H)	31.66	32.1
8	1.00 – 1.80	32.0	32.2
9	1.00 – 1.80	45.87	50.5
10	–	36.52	36.5
11	1.00 – 1.80	21.09	21.2
12	1.00 – 1.80	39.79	40.0
13	–	42.30	42.2
14	1.00 – 1.80	56.79	57.1
15	1.00 – 1.80	26.13	24.5
16	1.00 – 1.80	28.24	28.9
17	1.00 – 1.80	56.08	56.3
18	0.69 (s, 3H)	11.98	12.2
19	1.01 (s, 3H),	19.39	19.5
20	2.06 (m, 1H)	40.4	40.4
21	0.93 (d, *J*=6.6 Hz, 3H)	19.80	21.4
22	5.14 (dd, *J* = 15.6, 8.4 Hz, 1H)	138.3	138.3
23	5.01 (dd, *J* = 15.6, 8.4 Hz, 1H)	129.3	129.7
24	1.00 – 1.80	50.16	51.5
25	1.00 – 1.80	36.15	32.2
26	0.83 (d, *J*=6.6 Hz, 3H)	19.04	21.2
27	0.84 (d, *J*=6.6 Hz, 3H)	18.78	19.2
28	1.00 – 1.80	24.3	25.4
29	0.86 (t, *J*=7.8 Hz, 3H)	11.86	12.2

* Measurements were recorded in deuterated chloroform.

Table S2. ^{1}H and ^{13}C NMR data for compound **2**

Carbon No.	δ_H **2** (600 MHz*)	δ_C **2** (150 MHz)	δ_C (Krzyczkowski *et al.*, 2009)
1	1.94 (m, 2H)	34.90	34.7
2	1.95 (m, 2H)	30.33	30.1
3	3.98 (m, 1H)	66.69	66.5
4	2.10 (dd, *J* = 5.4, 2.4 Hz, H-4a)		
	1.70 (t, *J* = 2.4 Hz, H-4b)	37.14	36.9
5	–	79.64	79.4
6	6.25 (d, *J*=8.7Hz, 1H)	135.62	135.2
7	6.51 (d, *J*=8.7Hz, 1H)	130.96	130.7
8	–	82.37	82.1
9	1.00 – 1.80	51.08	51.1
10	–	39.96	39.3
11	1.00 – 1.80	20.84	20.6
12	1.00 – 1.80	39.55	39.7
13	–	44.77	44.6
14	1.00 – 1.80	51.69	51.7
15	1.00 – 1.80	23.61	23.4
16	1.00 – 1.80	28.87	28.6
17	1.00 – 1.80	56.41	56.2
18	0.83 (s, 3H)	13.09	12.9
19	0.89 (s, 3H)	17.77	18.2
20	2.0 (m, 1H)	37.17	36.9
21	1.01 (d, *J*=6.6Hz, 3H)	19.86	20.9
22	5.13 (dd, *J*= 15.6, 8.4 Hz, 1H)	135.41	135.4
23	5.20 (dd, *J*= 15.6, 8.4 Hz, 1H)	132.52	132.3
24	1.85 (m, 1H)	42.99	42.8
25	1.53 (m, 1H)	33.28	33.1
26	0.84 (d, *J*=7.2Hz, 3H)	20.16	19.6
27	0.82 (d, *J*=6.6Hz, 3H)	21.09	19.9
28	1.55 (d, *J*=7.2Hz, 3H)	18.39	17.6

* Measurements were recorded in deuterated chloroform.

d 12.9 (18-Me), 17.6 (28-Me), 18.2 (19-Me), 19.6 (26-Me), 19.9 (27-Me), 20.6 (11), 20.9 (21-Me), 23.4 (15), 28.6 (16), 30.1 (2), 33.1 (25), 34.7 (1), 36.9 (4), 36.9 (20), 39.3 (10), 39.7 (12), 42.8 (24), 44.6 (13), 51.1 (9), 51.7 (14), 56.2 (17), 66.5 (3), 79.4 (5), 82.1 (8), 130.7 (7), 132.3 (23), 135.2 (6), 135.4 (22).

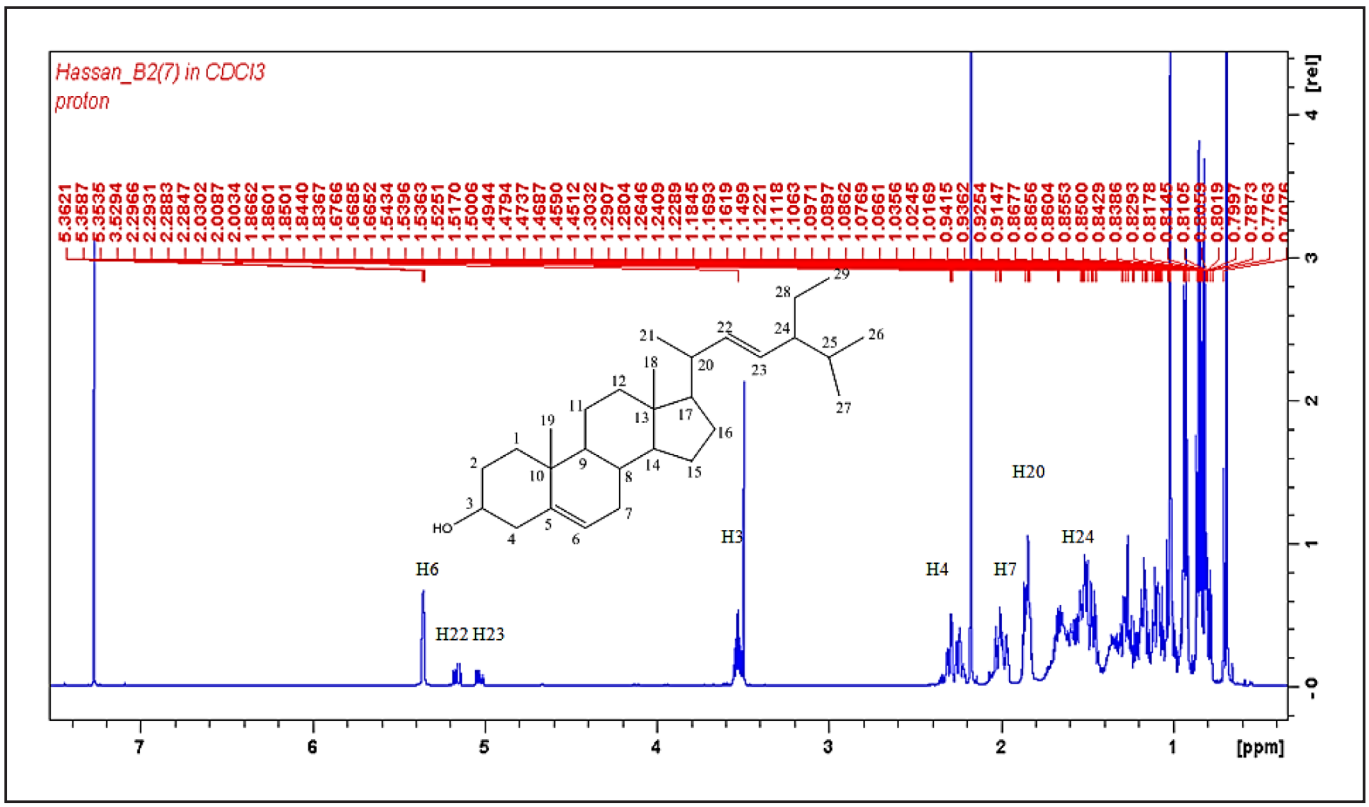


Figure S1a. ^{1}H NMR spectra of compound **1**.

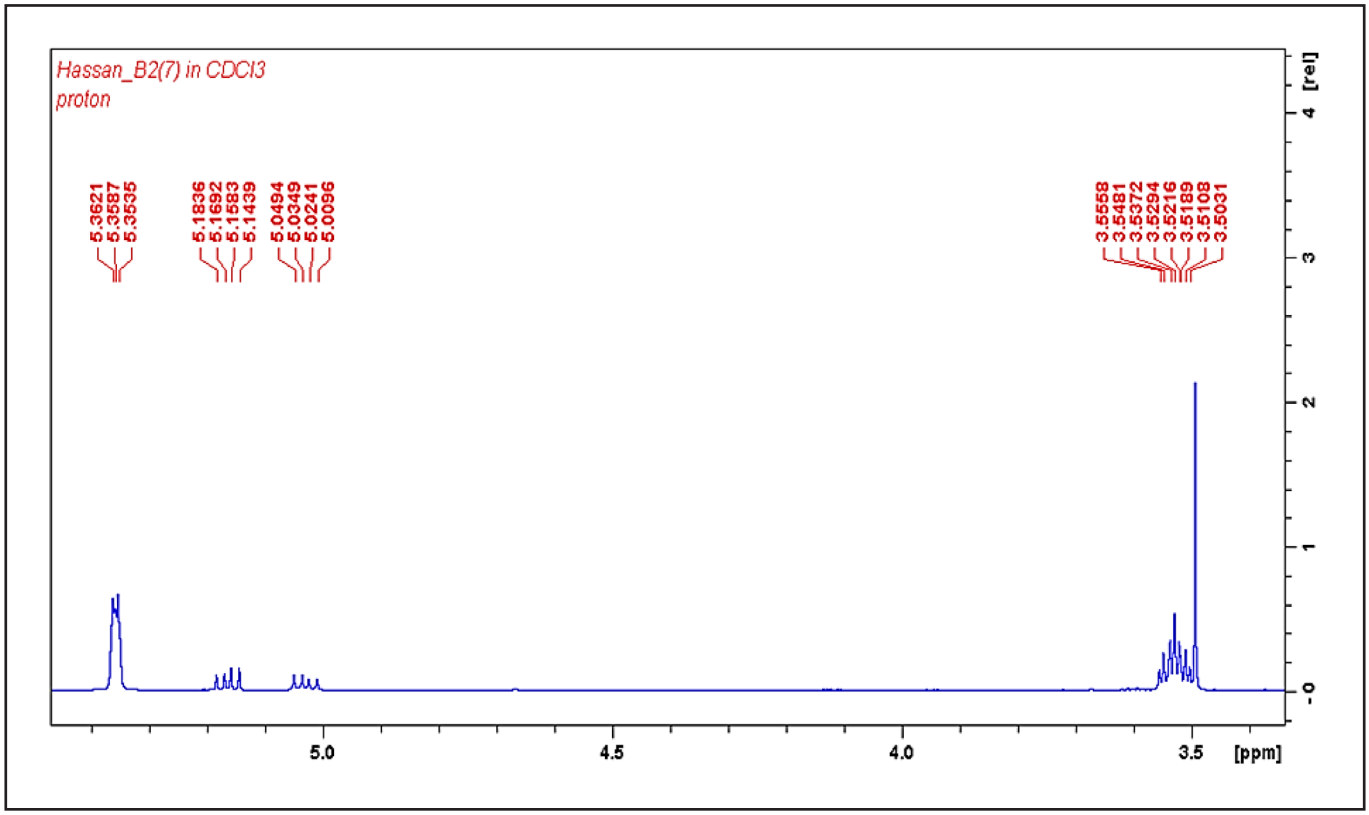


Figure S1b. ^{1}H NMR spectra of compound **1**.

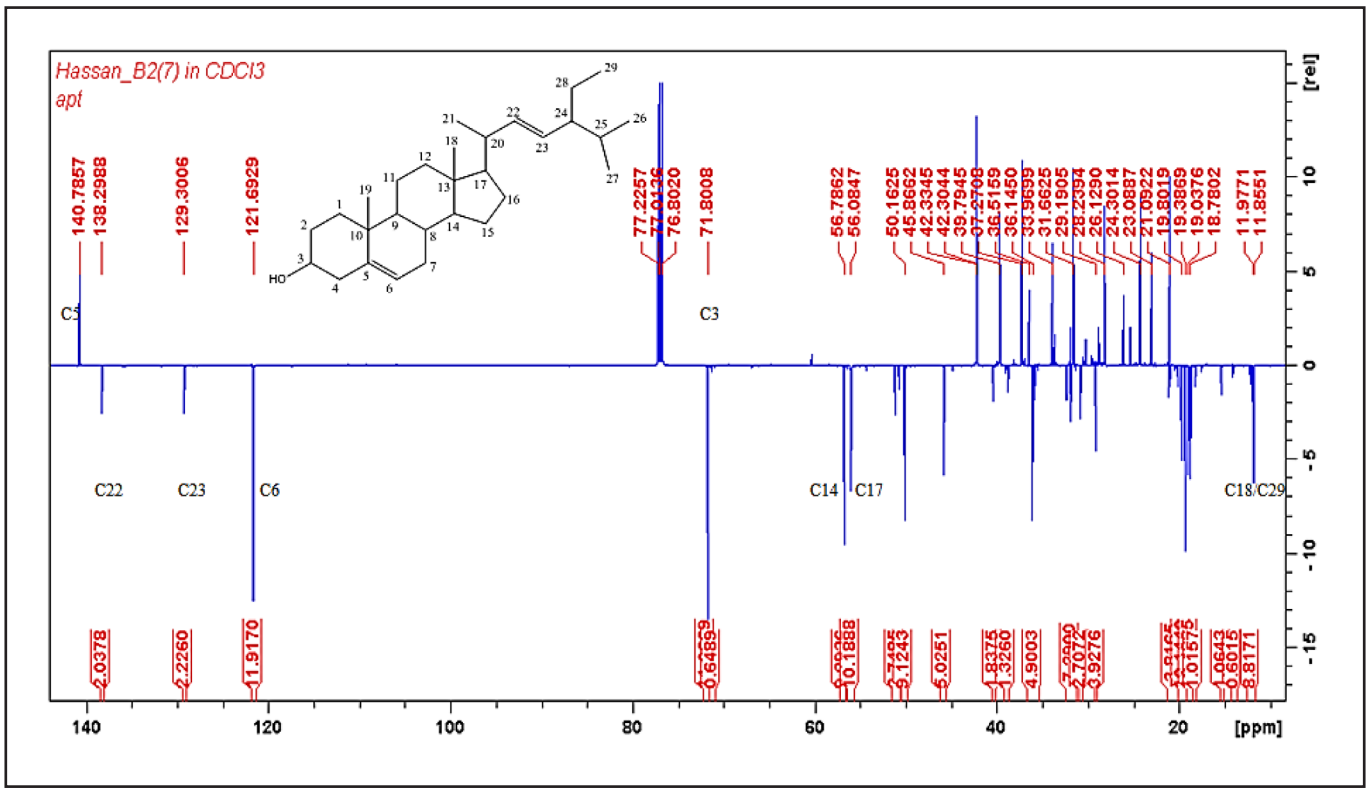


Figure S2. ^{13}C NMR spectra of compound **1**.

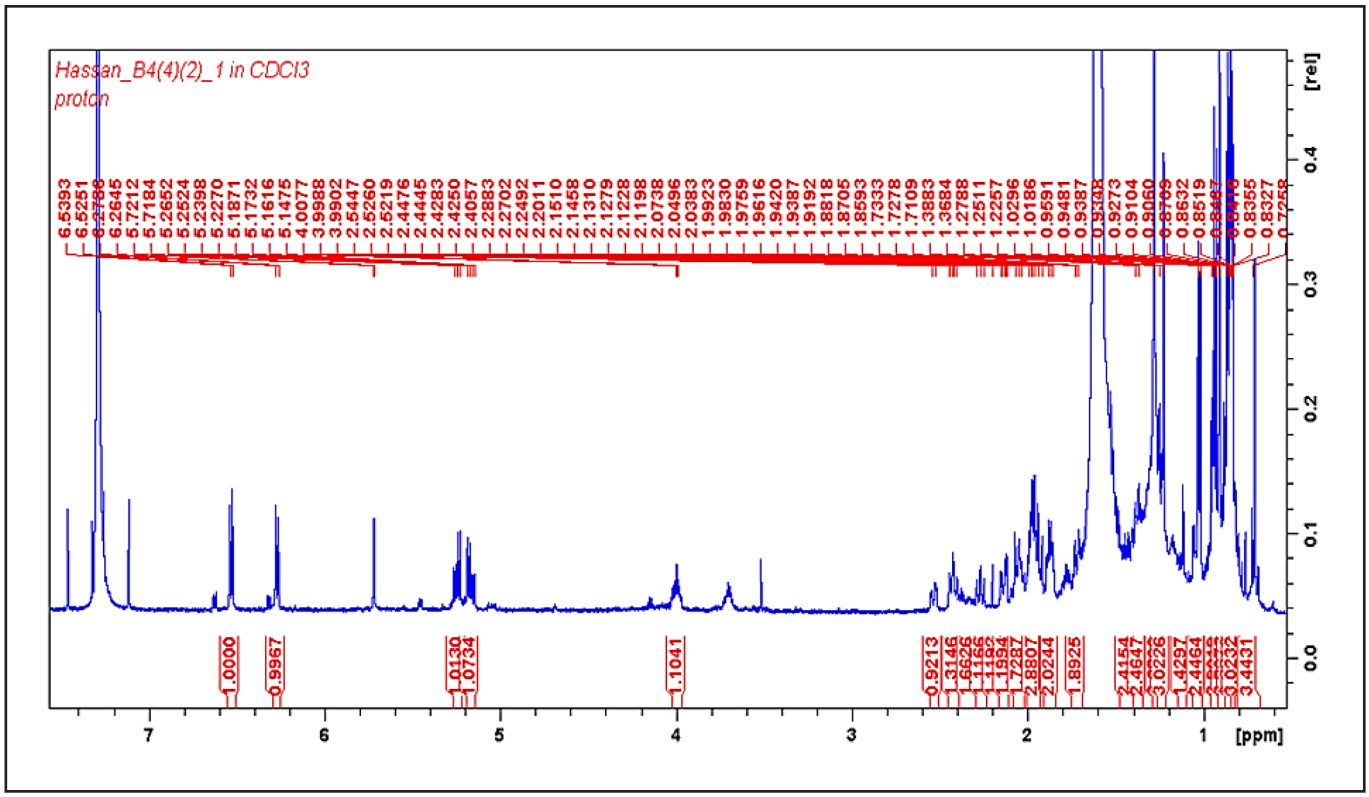


Figure S3a. ^{1}H NMR spectra of compound **2**.

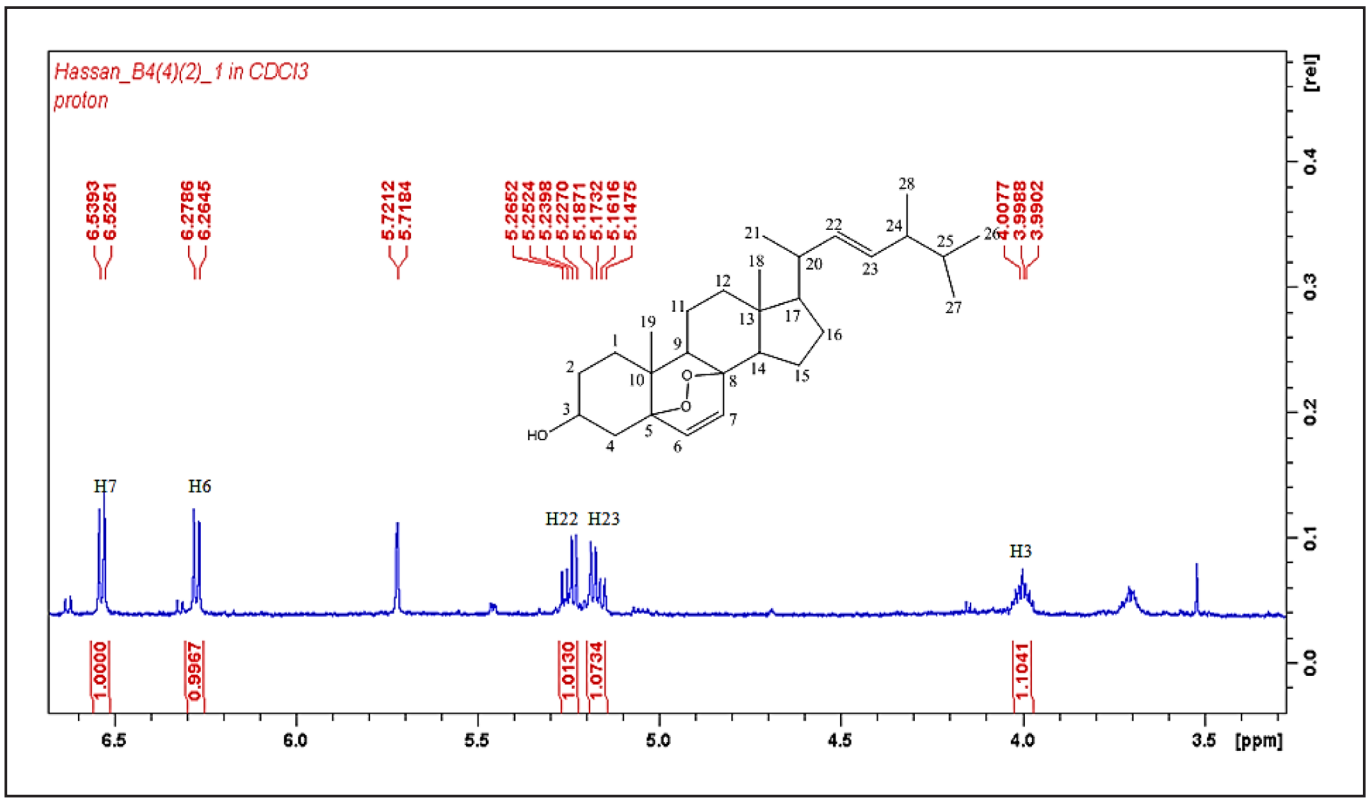


Figure S3b. ^{1}H NMR spectra of compound **2**.

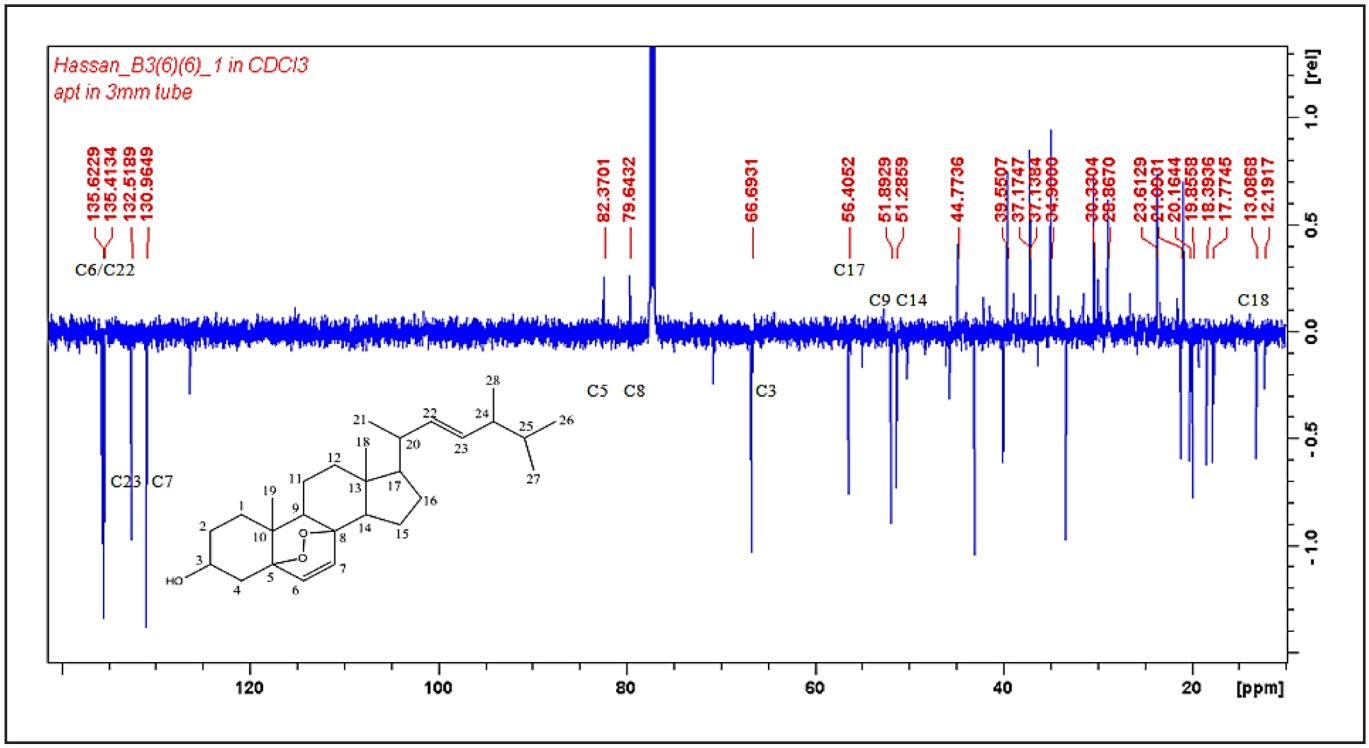
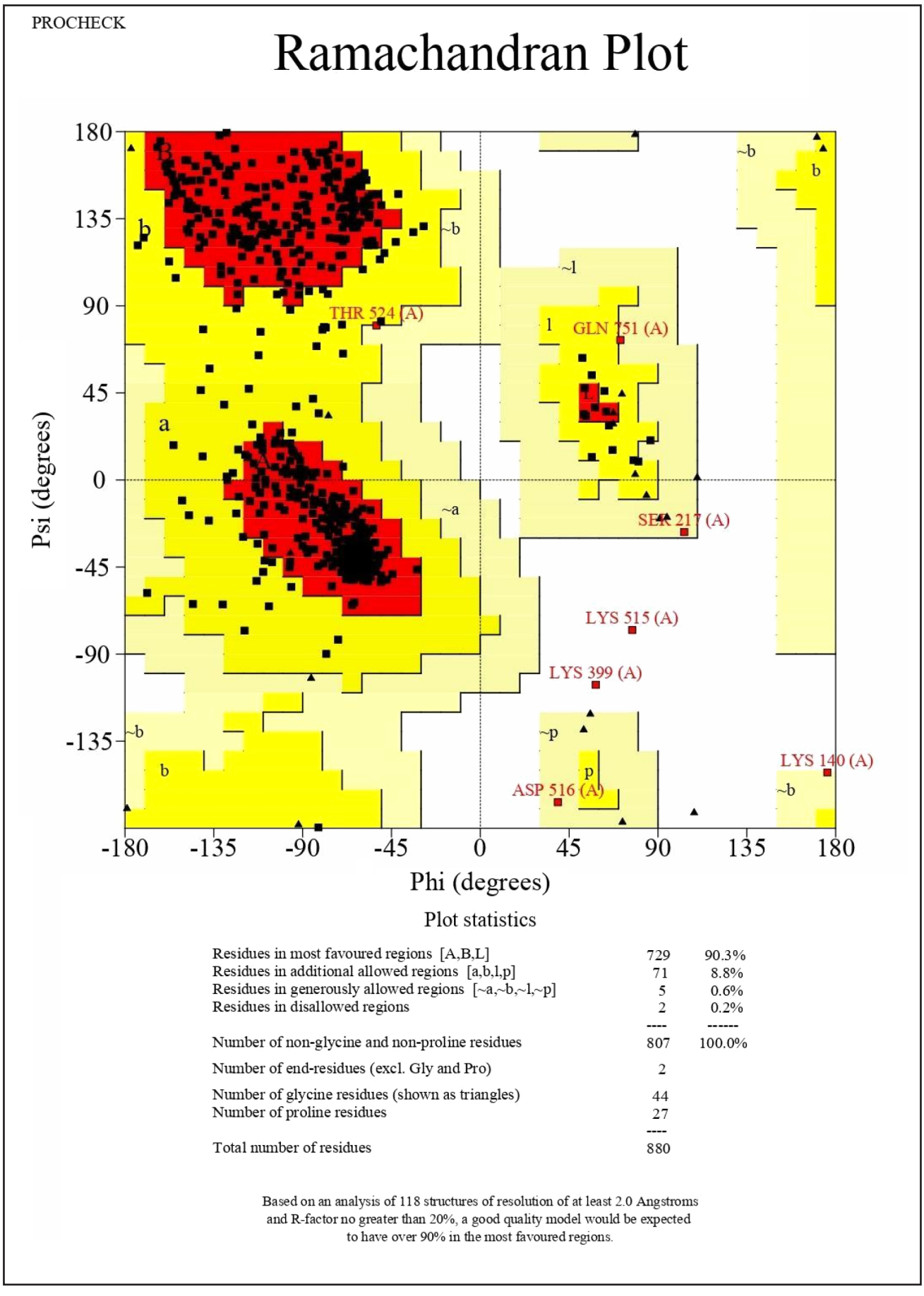


Figure S4. ^{13}C NMR spectra of compound **2**.



Plot statistics

Residues in most favoured regions [A,B,L]	729	90.3%
Residues in additional allowed regions [a,b,l,p]	71	8.8%
Residues in generously allowed regions [~a,~b,~l,~p]	5	0.6%
Residues in disallowed regions	2	0.2%
Number of non-glycine and non-proline residues	807	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	44	
Number of proline residues	27	
Total number of residues	880	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

9992547_01.ps

Figure S5. Ramachandaran plot analysis for a homology protein PfATP6.