The marine natural-derived inhibitors of glycogen synthase kinase-3β phenylmethylene hydantoins: In vitro and in vivo activities and pharmacophore modeling

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Table S1. ^{1}H NMR Data of Compounds **1**-**4** and **6**-**8.**[a]

Position	δ_H						
	1	**2**	**3**	**4**	**6**	**7**	**8**
1	10.36, brs	10.41, brs	10.38, brs	10.60, brs	10.54	10.20, brs	10.32, brs
2	11.17, brs	11.13, brs	11.04, brs	11.27, brs	11.23	11. 52, brs	11.04, brs
6	6.36, s	6.36, s	6.33, s	6.39, s	6.45, s	6.43, s	6.39, s
7	-	-	-	-	-	-	-
8	7.47, d (8.4)	7.56, d (8.4)	7.44, d (8.0)	7.19, d (8.0)	-	7.68, 2H, m	7.67, d (8.1)
9	6.78, d (8.4)	7.28, d (8.4)	6.65, d (8.0)	7.32, dd (8.0, 8.0)	7.68, m	7.66, 2H, m	7.47, d (8.1)
10	-	-	-	6.90, dd (8.6, 2.2)	7.40, m	-	-
11	6.78, d (8.4)	7.28, d (8.4)	6.65, d (8.0)	-	7.18, m	7.66, 2H, m	7.47, d (8.1)
12	7.47, d (8.4)	7.56, d (8.4)	7.44, d (8.0)	7.12, s	7.42, m	7.68, 2H, m	7.67, d (8.1)
1’	-	3.02, q (7.4)	-	-	-	-	
2’	-	1.23, t (7.4)	3.36, 2H, q (10.3)	3.83, 3H, s	-	-	
3’	-		1.09, 3H, t (7.0)		7.51, m	7.59, dd (5.1, 1.1)	
4’	-		3.36, 2H, q (10.3)		7.17, m	7.16, dd (5.1, 3.7)	
5’	-		1.09, 3H, t (7.0)		7.67, m	7.62, dd (3.7, 1.1)	
OH	9.98, brs						

[a]In DMSO, 400 MHz. Coupling constants (*J*) are in Hz.

Table S2. ^{13}C NMR Data of Compounds **1-4** and **6-8**.[a]

Position	δ_C						
	1	**2**	**3**	**4**	**6**	**7**	**8**
2	156.6, qC	156.6, qC	156.1 qC	155.8, qC	156.2, qC	156.3, qC	156.0, qC
4	166.7, qC	166.5, qC	166.3, qC	166.1, qC	165.9, qC	166.1, qC	165.8, qC
5	126.4, qC	137.8, qC	124.0, qC	129.2, qC	130.0, qC	128.4, qC	124.4, qC
6	110.4, CH	108.2, CH	111.1, CH	109.9, CH	107.1, CH	108.2, CH	107.3, CH
7	124.9, qC	128.3, qC	120.0, qC	135.5, qC	131.4, qC	132.6, qC	132.6, qC
8	132.3, CH	130.4, CH	131.9, CH	122.6, CH	134.5, qC	130.7, CH	129.2, CH
9	116.8, CH	127.8, CH	111.8, CH	130.6, CH	128.0, CH	126.0, CH	128.6, CH
10	159.0, CH	130.5, qC	148.1, qC	115.8, CH	129.2, CH	134.0, qC	133.8, qC
11	116.8, CH	127.8, CH	111.8, CH	160.1, qC	128.5, CH[b]	126.0, CH	128.6, CH
12	132.3, CH	130.4, CH	131.9, CH	115.0, CH	128.7, CH	130.7, CH	129.2, CH
1’		26.0, CH_2	40.5, CH_2	-	-	-	
2’		14.6, CH_3	13.0, CH_3	56.2, CH_3	141.5, qC	143.2, qC	
3’			40.5, CH_2		130.7, CH	126.8, CH	
4’			13.0, CH_3		128.6, CH[b]	129.2, CH	
5’					130.0, CH	124.9, CH	

[a]In DMSO, 100 MHz. Carbon multiplicities were determined by APT experiments. qC = quaternary, CH = methine carbons, CH_2 = methylene, CH_3 = methyl carbons.

Table S3. Mass and Melting Point Data of Compounds **1-4** and **6**-**8**.[40]

Compound No.	(M+1)	Melting Point (^{o}C)
1	205.5	311-314
2	248.1	222-225
3	260.5	256-258
4	219.1	178-180
6	270.0	247-250
7	270.0	299-301
8	232.2	303-305