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Supplementary Materials

Structural Characterization of Alzheimer DNA Promoter Sequences from Amyloid Precursor Gene in Presence of Thioflavin T and Analogs

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Table S1. Main characteristics of some of the selected and tested oligonucleotide sequences.

Name	Sequence (5′->3′)	MW (g/mol)	GC-content (%)	Extinction Coefficient (mol.cm)	Tm [°C]	Bases
PAD1_F	5′-AAATGAGGTGGAGAATGTA-3′	5965	36.8	240430	50.2	19
PAD1_R	5′-TACATTCTCCACCTCATTT-3′	5649	36.8	333460	50.2	19
PADS_F	5′-AATGAGGTGGAGAATGT-3′	5338	41	166980	48	17
PADS_R	5′-ACATTCTCCACCTCATT-3′	5040	41	282040	48	17
PADM_F	5′-AATGAGGTGGAGAAT-3′	3646	40	313040	42.4	15
PADM_R	5′-ATTCTCCACCTCATT-3′	3357	40	115440	42.4	15
PAD102	5′-TATACAGCTGTATA-3′	4261	29	251730	35	14
8ASH	5′-CCGGGGTACCCCGG-3′	4265	86	219380	58	14
ABCC1_F	5′-GCCCACCACGGC-3′	3576	83	231420	36	12
ABCC1_R	5′-GCCGTGGTGGGC-3′	3718	83	245110	32	12
1QV4*	5′-CGTGAATTCACG-3′	3645	50	111900	36	12
PADL1	5′-AACAGCTGTT-3′′	3027	40	332700	28	10

* used as control.

Table S2. Selected bond lengths and angles for **2** and **3.**

2			**3**		
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
S1	C6	1.730(2)	S1	C6	1.735(7)
S1	C7	1.754(2)	S1	C7	1.737(7)
N1	C5	1.382(2)	N1	C7	1.349(8)
N1	C7	1.294(3)	N1	C5	1.402(8)
N2	C7	1.384(3)	N1	C18	1.475(8)
N2	C8	1.293(3)	N2	C7	1.319(8)
N3	C12	1.362(3)	N2	C8	1.306(9)
N3	C16	1.441(3)	N3	C12	1.350(8)

2			3		
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
N3	C15	1.451(3)	N3	C16	1.461(9)
C5	C6	1.410(3)	N3	C15	1.439(8)
C5	C4	1.388(3)	C9	C14	1.417(9)
C6	C1	1.392(3)	C9	C8	1.405(9)
C9	C8	1.435(3)	C9	C10	1.405(9)
C9	C14	1.405(3)	C12	C13	1.421(9)
C9	C10	1.397(3)	C12	C11	1.425(9)
C3	C4	1.370(3)	C6	C1	1.384(9)
C3	C2	1.405(3)	C6	C5	1.392(9)
C11	C12	1.404(3)	C13	C14	1.368(9)
C11	C10	1.369(3)	C1	C2	1.395(10)
C12	C13	1.417(3)	C11	C10	1.351(9)
C1	C2	1.380(3)	C2	C3	1.407(10)
C14	C13	1.365(3)	C2	C17	1.493(10)
C2	C17	1.508(3)	C3	C4	1.371(10)
			C5	C4	1.371(9)
			N31	C31	1.105(16)
			C30	C31	1.441(18)

2				3			
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C6	S1	C7	88.99(10)	C6	S1	C7	91.2(3)
C7	N1	C5	110.53(18)	C7	N1	C5	114.5(6)
C8	N2	C7	116.8(2)	C7	N1	C18	122.5(6)
C12	N3	C16	121.3(2)	C5	N1	C18	123.0(6)
C12	N3	C15	121.2(2)	C8	N2	C7	121.1(6)
C16	N3	C15	117.0(2)	C12	N3	C16	122.2(6)
N1	C5	C6	115.45(18)	C12	N3	C15	121.7(6)
N1	C5	C4	126.0(2)	C15	N3	C16	116.0(6)
C4	C5	C6	118.58(19)	C8	C9	C14	121.3(7)
C5	C6	S1	109.02(15)	C10	C9	C14	117.1(6)
C1	C6	S1	129.75(18)	C10	C9	C8	121.6(7)
C1	C6	C5	121.2(2)	N3	C12	C13	121.7(6)
N1	C7	S1	116.00(15)	N3	C12	C11	120.6(6)
N1	C7	N2	129.1(2)	C13	C12	C11	117.6(6)
N2	C7	S1	114.93(16)	C1	C6	S1	129.1(5)
C14	C9	C8	122.4(2)	C1	C6	C5	119.8(6)
C10	C9	C8	120.3(2)	C5	C6	S1	111.0(5)
C10	C9	C14	117.3(2)	C14	C13	C12	120.5(6)
N2	C8	C9	122.6(2)	C6	C1	C2	119.5(7)
C4	C3	C2	121.9(2)	C13	C14	C9	121.6(7)
C10	C11	C12	121.2(2)	N1	C7	S1	111.3(5)
N3	C12	C11	121.9(2)	N2	C7	S1	128.2(5)
N3	C12	C13	121.2(2)	N2	C7	N1	120.5(6)
C11	C12	C13	116.97(19)	N2	C8	C9	122.3(7)
C3	C4	C5	119.8(2)	C10	C11	C12	120.7(6)
C2	C1	C6	119.6(2)	C1	C2	C3	118.5(6)
C13	C14	C9	121.3(2)	C1	C2	C17	121.0(7)
C3	C2	C17	120.4(2)	C3	C2	C17	120.4(7)
C1	C2	C3	118.8(2)	C4	C3	C2	122.3(7)

2				**3**			
Atom	**Atom**		**Length/Å**	**Atom**	**Atom**		**Length/Å**
C1	C2	C17	120.8(2)	C6	C5	N1	111.9(6)
C11	C10	C9	121.8(2)	C4	C5	N1	126.1(6)
C14	C13	C12	121.4(2)	C4	C5	C6	122.0(6)
				C11	C10	C9	122.5(7)
				C3	C4	C5	117.9(7)
				N31	C31	C30	176.0(16)

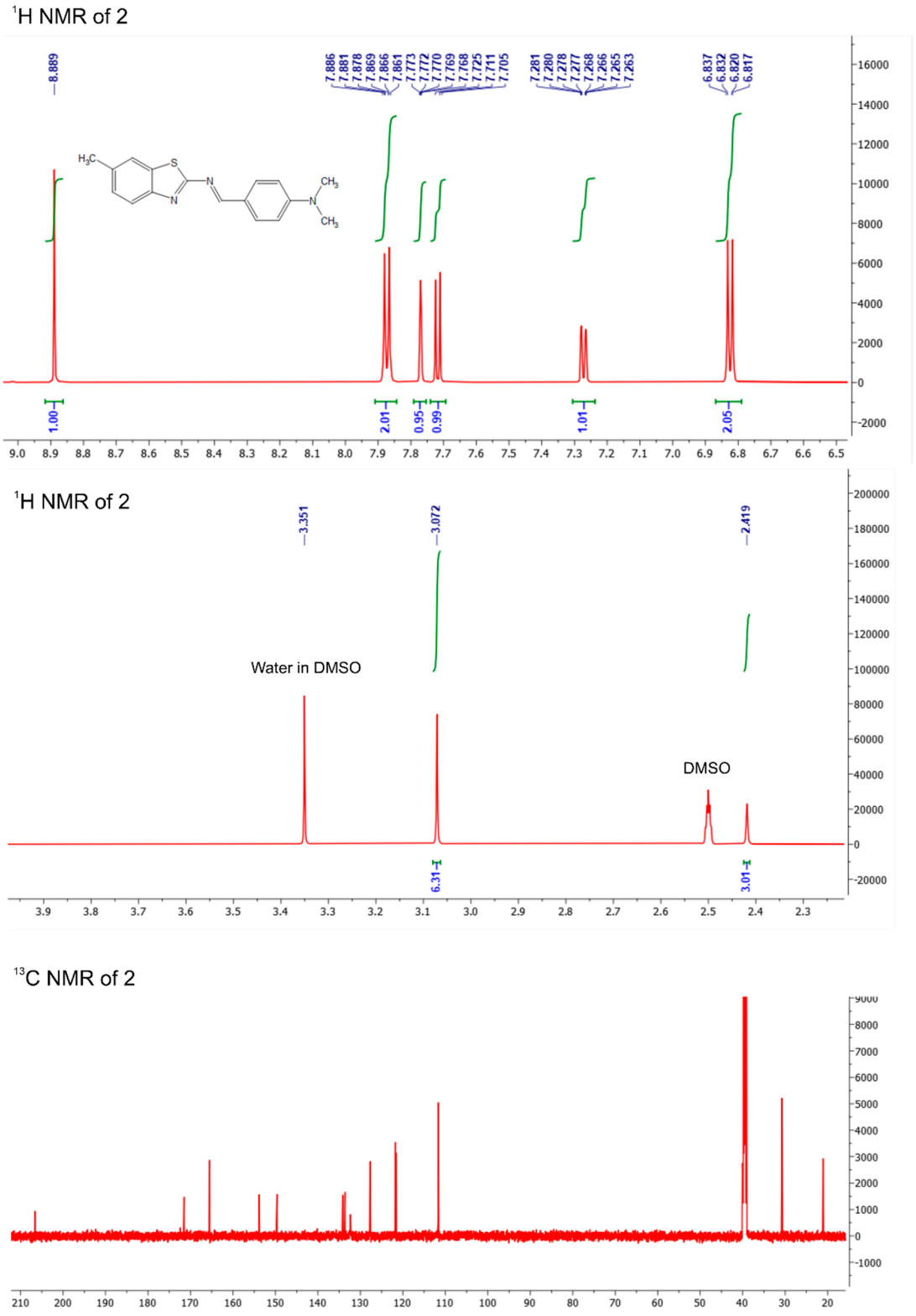

Figure S1. ^{1}H and ^{13}C NMRs of compound **2.**

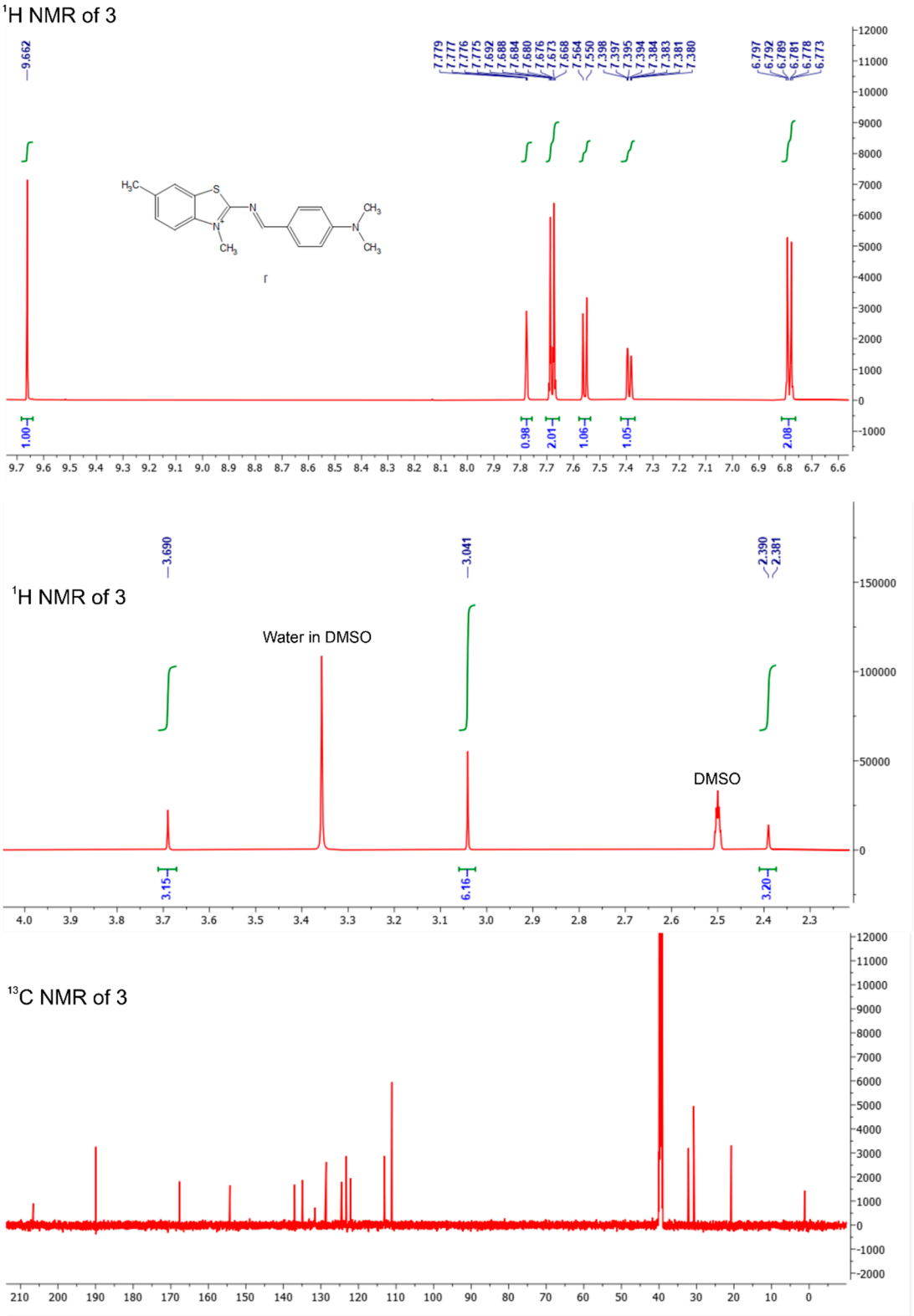

Figure S2. ^{1}H and ^{13}C NMRs of compound **3.**

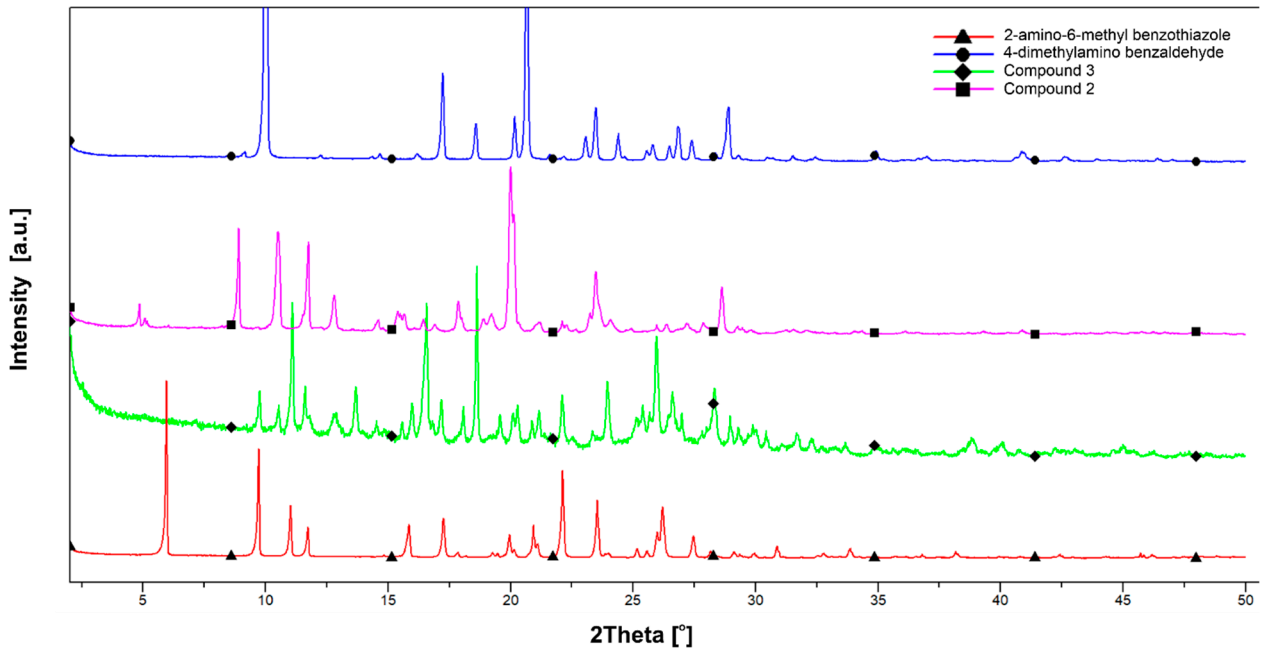

Figure S3. Comparison of the X-ray powder diffraction patterns of the starting and synthesized compounds **2** and **3**.