SUPPLEMENTARY MATERIALS

2,7-bis(pyridin-4-ylethynyl)-9H-carbazole

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Figure S1: FT-IR spectrum (4000–400 cm^{-1}) recorded for compound **1** (KBr pellet).

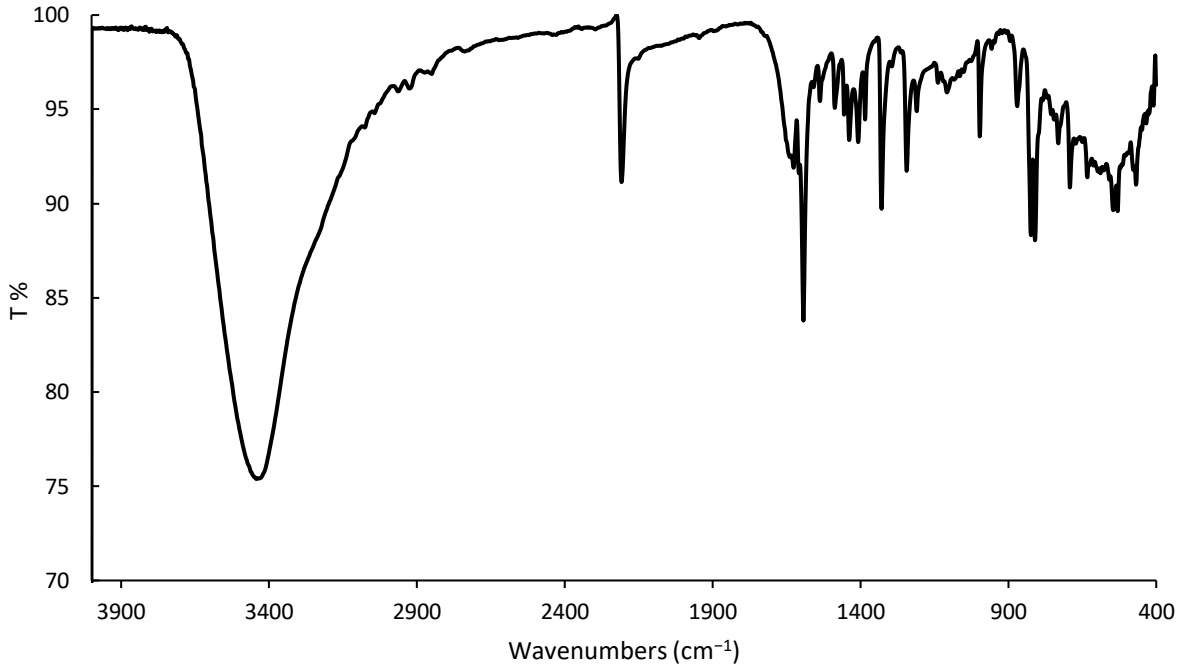

Figure S2: ^{1}H NMR (600 MHz, DMSO-d_6) spectrum recorded for compound **1**.

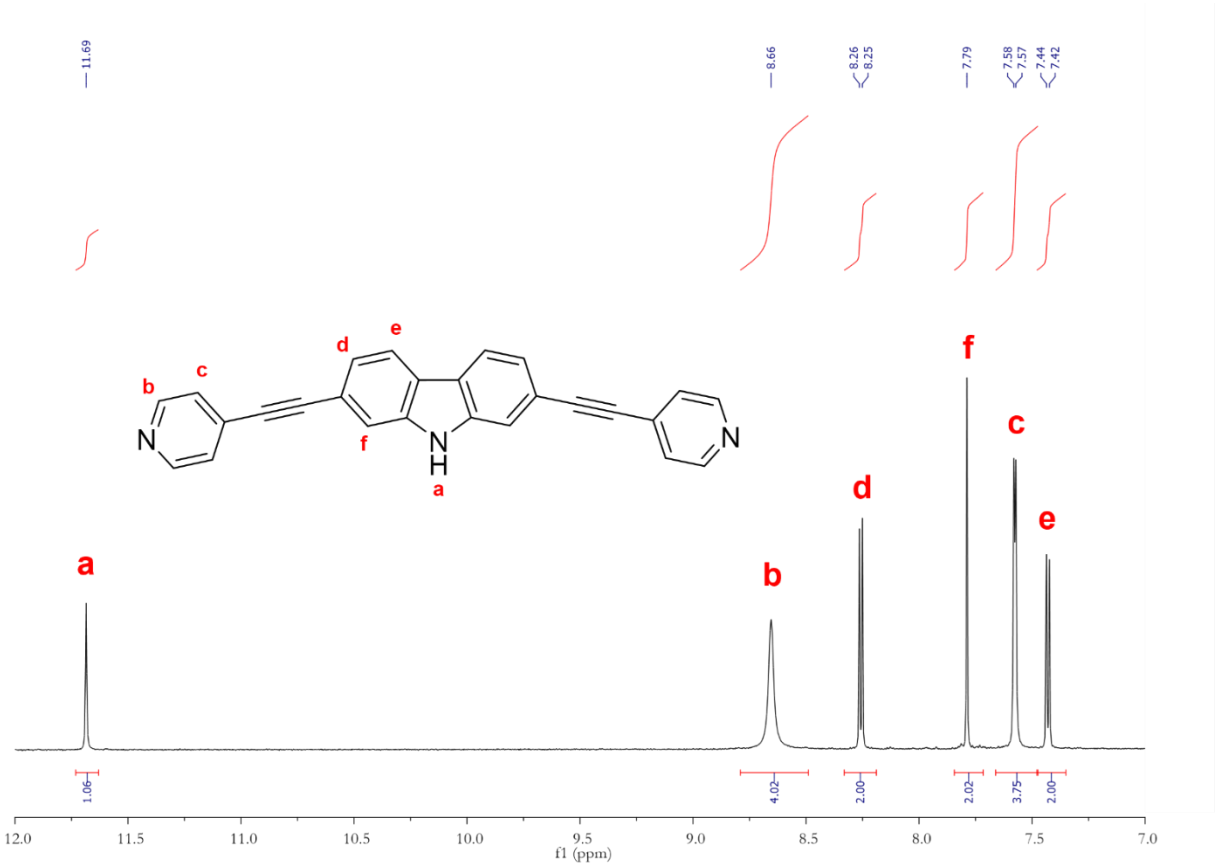

Figure S3: $^{13}C\{^{1}H\}$ NMR (151 MHz, DMSO-d_6) spectrum recorded for compound **1.**

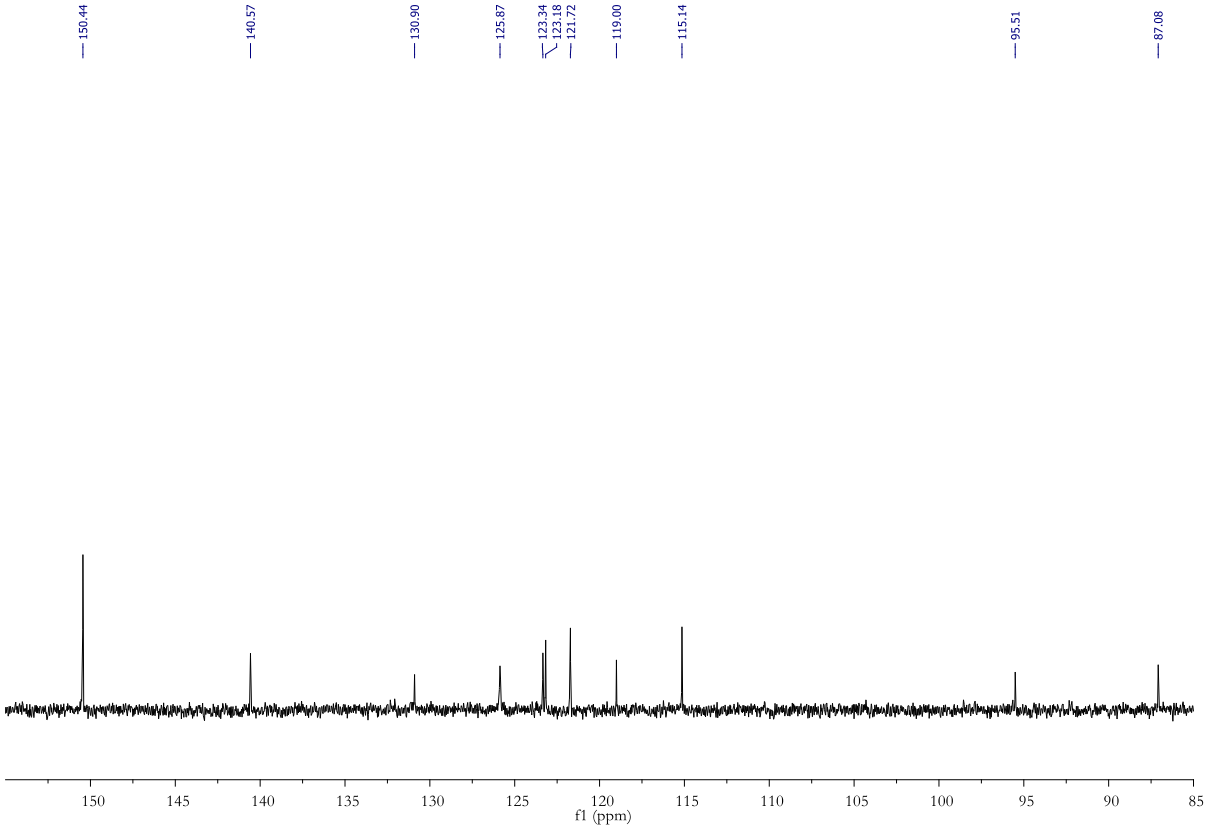

Figure S4: ESI(+) MS spectrum recorded for compound **1**.

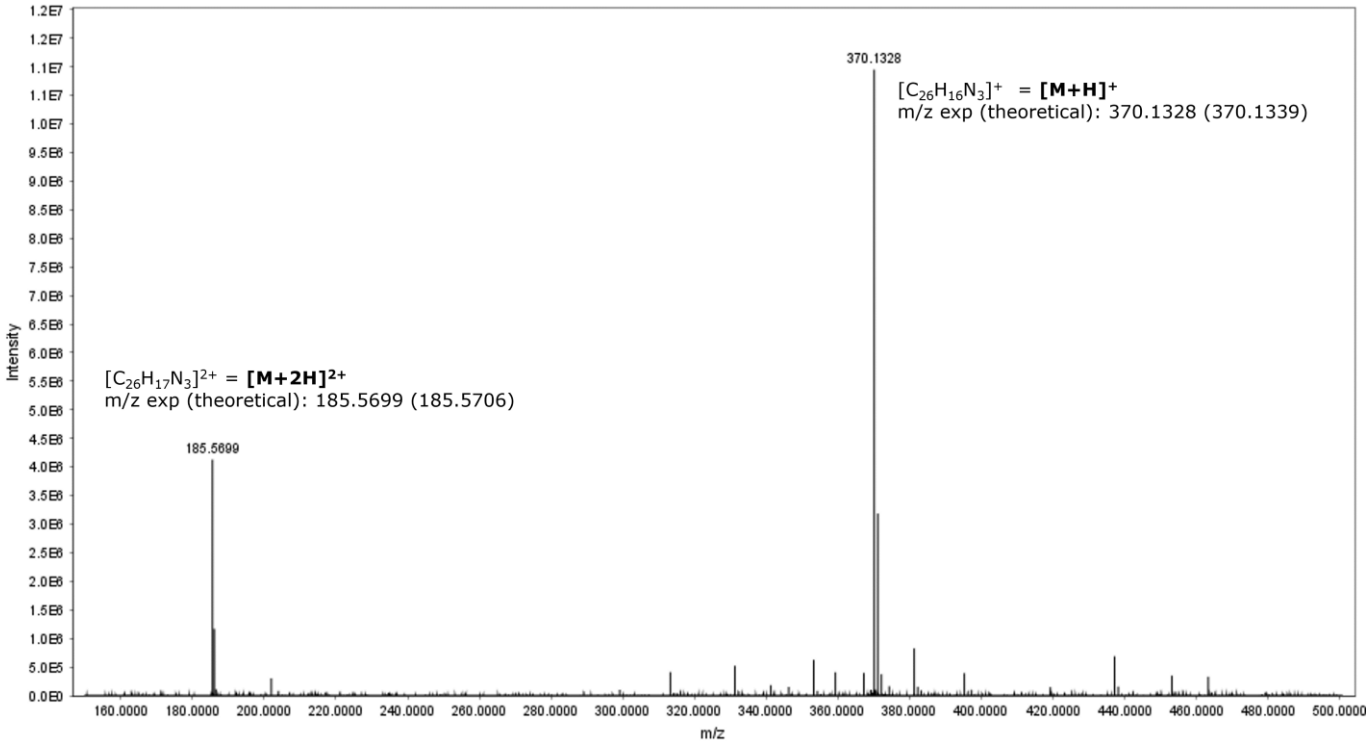

Table S1: Crystal data and refinement parameters for compound **1·H$_2$O**.

Formula	$C_{26}H_{17}N_3O$
$D_{calc.}$/ g cm^{-3}	1.276
μ/mm^{-1}	0.629
Formula Weight (g mol^{-1})	387.42
Colour	colourless
Shape	(cut) block
Size/mm^3	0.144×0.070×0.040
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	9.0349(3)
b/Å	25.4077(7)
c/Å	17.7142(4)
α/°	90
β/°	97.260(3)
γ/°	90
V/Å^3	4033.8(2)
Z	8
Z'	2
Wavelength/Å	1.54178
Radiation type	Cu $K\alpha$
Θ_{min}/°	3.058
Θ_{max}/°	68.241
Measured Refl.	37690
Independent Refl.	7385
Reflections with I > 2(I)	6168
R_{int}	0.0562
Parameters	553
Restraints	0
Largest Peak	0.665
Deepest Hole	-0.376
GooF	1.162
wR_2 (all data)	0.2459
wR_2	0.2352
R_1 (all data)	0.1035
R_1	0.0907

Table S2: Bond lengths (Å) for compound **1·H₂O**.

Atom	Atom	Length/Å
C1	C2	1.382(4)
C1	C6	1.416(4)
C2	C3	1.402(4)
C3	C4	1.420(4)
C3	C16	1.439(4)
C4	C5	1.393(4)
C4	N1	1.381(4)
C5	C6	1.391(4)
C6	C7	1.434(4)
C7	C8	1.205(4)
C8	C9	1.424(4)
C9	C10	1.399(4)
C9	C13	1.393(4)
C10	C11	1.373(4)
C11	N2	1.344(4)
C12	C13	1.374(4)
C12	N2	1.332(4)
C14	C15	1.378(4)
C14	C19	1.406(4)
C15	C16	1.395(4)
C16	C17	1.420(4)
C17	C18	1.384(4)
C17	N1	1.387(4)
C18	C19	1.394(4)
C19	C20	1.440(4)
C20	C21	1.197(4)
C21	C22	1.434(4)
C22	C23	1.393(5)
C22	C26	1.396(4)
C23	C24	1.387(5)
C24	N3	1.333(5)
C25	C26	1.380(4)
C25	N3	1.333(4)
C27	C28	1.376(4)
C27	C32	1.407(4)
C28	C29	1.400(4)
C29	C30	1.422(4)
C29	C42	1.436(4)
C30	C31	1.382(4)
C30	N4	1.378(4)
C31	C32	1.393(4)
C32	C33	1.438(4)
C33	C34	1.198(4)
C34	C35	1.432(4)
C35	C36	1.392(4)
C35	C39	1.402(4)
C36	C37	1.386(4)
C37	N5	1.334(4)
C38	C39	1.379(4)
C38	N5	1.340(4)
C40	C41	1.378(4)
C40	C45	1.411(4)
C41	C42	1.403(4)
C42	C43	1.415(4)
C43	C44	1.388(4)
C43	N4	1.383(4)
C44	C45	1.393(4)
C45	C46	1.443(4)
C46	C47	1.193(4)
C47	C48	1.436(4)
C48	C49	1.391(4)
C48	C52	1.402(4)
C49	C50	1.377(4)
C50	N6	1.351(4)
C51	C52	1.378(4)
C51	N6	1.332(4)

Table S3: Bond angles (°) for compound **1·H₂O**.

Atom	Atom	Atom	Angle/°
C2	C1	C6	120.2(3)
C1	C2	C3	119.6(3)
C2	C3	C4	119.1(3)
C2	C3	C16	134.4(3)
C4	C3	C16	106.4(2)
C5	C4	C3	122.0(3)
N1	C4	C3	109.3(2)
N1	C4	C5	128.6(3)
C6	C5	C4	117.4(3)
C1	C6	C7	118.3(3)
C5	C6	C1	121.6(3)
C5	C6	C7	120.0(3)
C8	C7	C6	177.9(3)
C7	C8	C9	178.4(3)
C10	C9	C8	121.0(3)
C13	C9	C8	121.4(3)
C13	C9	C10	117.6(3)
C11	C10	C9	119.0(3)
N2	C11	C10	123.8(3)
N2	C12	C13	124.7(3)
C12	C13	C9	118.6(3)
C15	C14	C19	121.2(3)
C14	C15	C16	119.1(3)
C15	C16	C3	134.0(3)
C15	C16	C17	119.1(3)
C17	C16	C3	106.8(2)
C18	C17	C16	122.0(3)
C18	C17	N1	129.1(3)
N1	C17	C16	108.9(2)
C17	C18	C19	117.7(3)
C14	C19	C20	118.8(3)
C18	C19	C14	120.8(3)
C18	C19	C20	120.4(3)
C21	C20	C19	177.9(3)
C20	C21	C22	178.0(3)
C23	C22	C21	121.8(3)
C23	C22	C26	117.3(3)
C26	C22	C21	120.8(3)
C24	C23	C22	119.0(3)
N3	C24	C23	123.6(3)
N3	C25	C26	123.8(3)
C25	C26	C22	119.1(3)
C28	C27	C32	121.1(3)
C27	C28	C29	119.5(3)
C28	C29	C30	118.7(3)
C28	C29	C42	134.8(3)
C30	C29	C42	106.4(2)
C31	C30	C29	121.8(3)
N4	C30	C29	109.1(2)
N4	C30	C31	129.1(3)
C30	C31	C32	118.2(3)
C27	C32	C33	118.9(3)
C31	C32	C27	120.6(3)
C31	C32	C33	120.5(3)
C34	C33	C32	177.9(3)
C33	C34	C35	176.2(3)
C36	C35	C34	122.5(3)
C36	C35	C39	117.3(3)
C39	C35	C34	120.1(3)
C37	C36	C35	118.8(3)
N5	C37	C36	124.1(3)
N5	C38	C39	123.5(3)
C38	C39	C35	119.4(3)
C41	C40	C45	120.6(3)
C40	C41	C42	119.5(3)
C41	C42	C29	134.4(3)
C41	C42	C43	118.9(3)
C43	C42	C29	106.7(2)
C44	C43	C42	122.2(3)
N4	C43	C42	109.1(2)
N4	C43	C44	128.6(3)
C43	C44	C45	117.6(3)
C40	C45	C46	119.3(3)
C44	C45	C40	121.2(3)
C44	C45	C46	119.5(3)
C47	C46	C45	178.2(3)
C46	C47	C48	176.4(3)
C49	C48	C47	121.5(3)
C49	C48	C52	117.5(3)
C52	C48	C47	121.0(3)
C50	C49	C48	119.1(3)
N6	C50	C49	123.9(3)
N6	C51	C52	124.4(3)
C51	C52	C48	118.8(3)
C4	N1	C17	108.7(2)
C12	N2	C11	116.3(3)
C25	N3	C24	117.1(3)
C30	N4	C43	108.7(2)
C37	N5	C38	116.8(3)
C51	N6	C50	116.3(3)