Supplementary Information

Influence of solvation on the spectral, molecular structure, and antileukemic activity of 1-benzyl-3-hydroxy-2-methylpyridin-4(1H)-one

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Table S1: Crystal data of 1-benzyl-3-hydroxy-2-methylpyridin-4(1H)-one (**BHM**).

Crystallographic data	4-MeTPh (BHM)
Emperical formula	$C_{14}H_{12}NO_2$
Formula weight (g mol^{-1})	215.74
Crystal system	Monoclinic
Space group	*P 21/c*
a (Å)	6.9245(2)
b (Å)	7.2365(2)
c (Å)	21.5135(7)
α (°)	90
β (°)	90
$_\gamma$(°)	90
Volume (Å^{-3})	1074.43(6)
Z	4
***P$_{calc}$* (g cm^{-3})**	1.334
Crystal colour	pale yellow
Crystal morphology	block
Crystal size (mm)	0.142 x 0.188 x 0.231
μ (mm^{-1})	0.089
F (000)	455
θ range (°)	1.90 -31.06
Index ranges	$-9 \leq h \leq 8$ $-10 \leq k \leq 10$

	$-30 \leq l \leq 28$
Reflections collected	20766
Unique reflections	2987
Reflection with I>2σ	2559
R_{int}	0.0535
Completeness to 2 theta (°, %)	25.24,100
Data/ restraints/ parameters	2987/0/147
GooF	1.082
R[I>2σ(I)]	R_1= 0.0544 wR_2 = 0.1439
R(all data)	R_1= 0.0616 wR_2 = 0.1474
ρ_{max} and ρ_{min} (e.Å^{-3})	0.454 and -0.208

Table S2: Selected bond lengths (Å) and angles (°) for BHM.

Description	Value	Description	Value	Description	Value
Bond lengths (Å)					
N1 C6	1.3835(19)	C6 C16	1.496(2)	N1 C2	1.354(2)
C8 C7	1.513(2)	N1 C7	1.4705(18)	C8 C9	1.387(2)
O1 C4	1.2645(18)	C8 C13	1.387(2)	C5 C4	1.440(2)
C9 C10	1.388(3)	C5 C6	1.367(2)	C13 C12	1.394(3)
C5 O2	1.3575(18)	C10 C11	1.380(3)	C4 C3	1.423(2)
C11 C12	1.370(3)	C3 C2	1.359(2)	N1 C6	1.3835(19)
C6 C16	1.496(2)	N1 C2	1.354(2)	C8 C7	1.513(2)
Bond angles (°)					
C6 N1 C7	120.42(13)	C5 C6 C16	122.18(13)	C13 C8 C9	119.12(16)
C2 N1 C6	120.35(13)	C9 C8 C7	118.74(15)	N1 C2 C3	122.50(14)
C2 N1 C7	119.22(13)	C13 C8 C7	122.08(15)	N1 C7 C8	113.89(13)
C6 C5 C4	122.43(14)	O1 C4 C5	120.44(14)	C8 C9 C10	120.49(17)
O2 C5 C4	118.10(13)	O1 C4 C3	124.34(14)	C8 C13 C12	119.75(18)
O2 C5 C6	119.46(13)	C3 C4 C5	115.21(13)	C11 C10 C9	120.23(17)
C2 C3 C4	120.49(14)	C5 C6 C16	122.18(13)	C12 C11 C10	119.51(18)
N1 C6 C16	118.87(13)	C9 C8 C7	118.74(15)	C11 C12 C13	120.90(19)
C5 C6 N1	118.95(13)	C13 C8 C7	122.08(15)	C6 N1 C7	120.42(13)
C13 C8 C9	119.12(16)	C2 N1 C6	120.35(13)	O2 C5 C4	118.10(13)
N1 C2 C3	122.50(14)	C2 N1 C7	119.22(13)	O2 C5 C6	119.46(13)
N1 C7 C8	113.89(13)	C6 C5 C4	122.43(14)	O1 C4 C5	120.44(14)
C8 C9 C10	120.49(17)	O1 C4 C3	124.34(14)	C11 C10 C9	120.23(17)
C8 C13 C12	119.75(18)	C3 C4 C5	115.21(13)		
Torsion angles (°)					
C6-N1-C2-C3	-1.25(14)	C7-N1-C2-C3	177.46(14)	O1-C4-C5-C6	177.45(14)
C3-C4-C5-O2	177.56(13)	C6-N1-C7-C8	-72.48(14)	C2-N1-C7-C8	108.81(14)
C4-C5-C6-C16	-177.82(16)	C7-N1-C6-C16	1.41(16)	C7-N1-C6-C5	-178.08(13)
O2-C5-C6-N1	-179.04(16)	N1-C2-C3-C4	-0.40(14)	C7-C8-C9-C10	176.70(14)
N1-C7-C8-C13	-35.97(13)	C2-C3-C4-O1	-178.13(16)	C2-N1-C6-C5	0.61(16)
C4-C5-C6-N1	1.65(14)	C2-C3-C4-C5	2.46(13)	C3-C4-C5-C6	-3.12(16)
N1-C7-C8-C9	146.78(14)	O1-C4-C5-O2	-1.87(14)	C7-C8-C13-C12	-176.70(14)

Table S3: Hydrogen bonds (Å, °) for BHM.

Description	D-H (Å)	H…A (Å)	D-H…A (Å)	D-H…A (°)	Symmetry code
O2-H2A…O1	0.8400	2.2700	2.7221	114.00	
O2-H2A…O1	0.8400	1.9400	2.7060	152.00	-x, -y, -z
C3-H3…O1	0.9500	2.3600	3.2926	166.00	-x, 1-y, -z

C7-H7B…O1	0.9900	2.4000	3.3644	165.00	1+x, y, z
C16-H16A…O1	0.9800	2.5300	3.4794	163.00	1+x, y, z
C16-H16B…O2	0.9800	2.3900	2.8333	107.00	

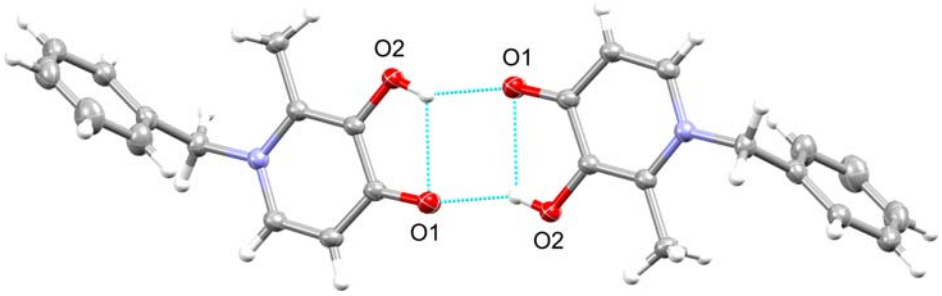

Figure S1: Hydrogen bonding present within BHM indicated using dotted cyan lines.

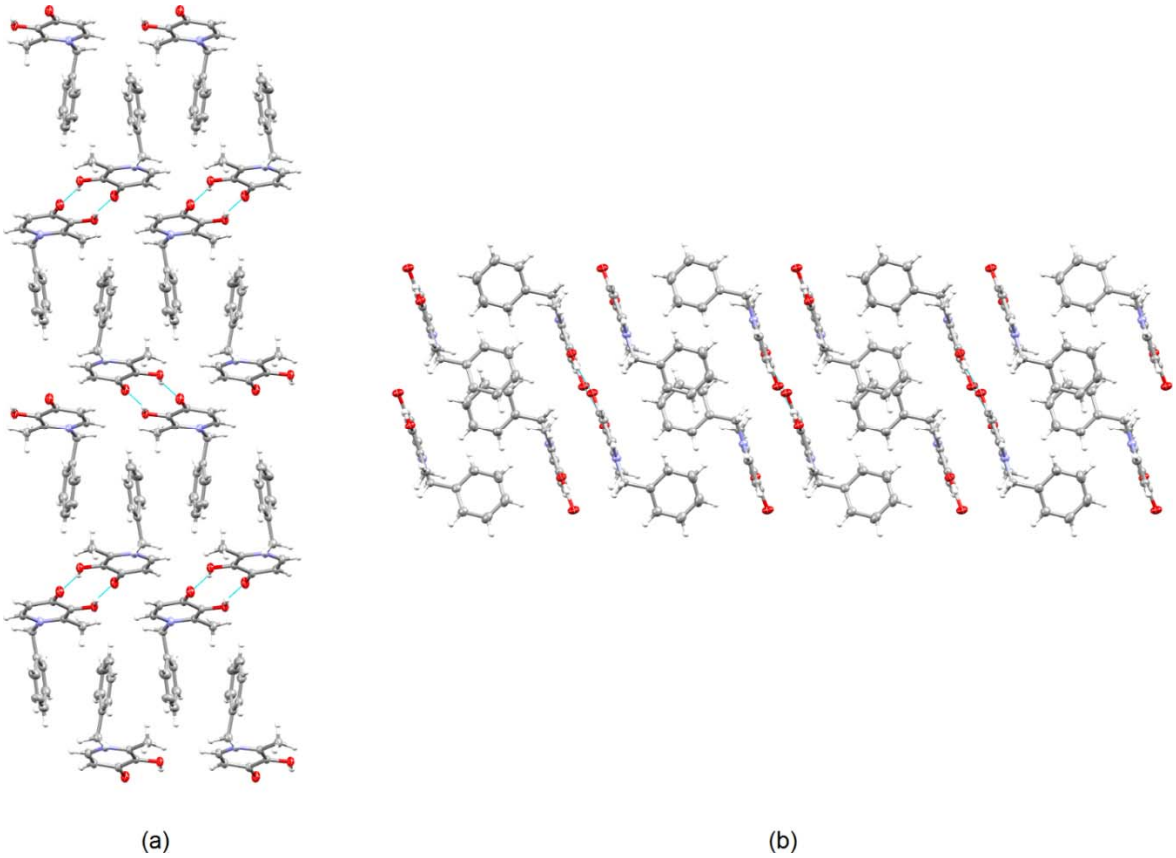

Figure S2: Packing diagrams of BHM when viewed along the (a) *a* axis and (b) *b* axis. Hydrogen bonds are indicated by the dotted cyan lines.

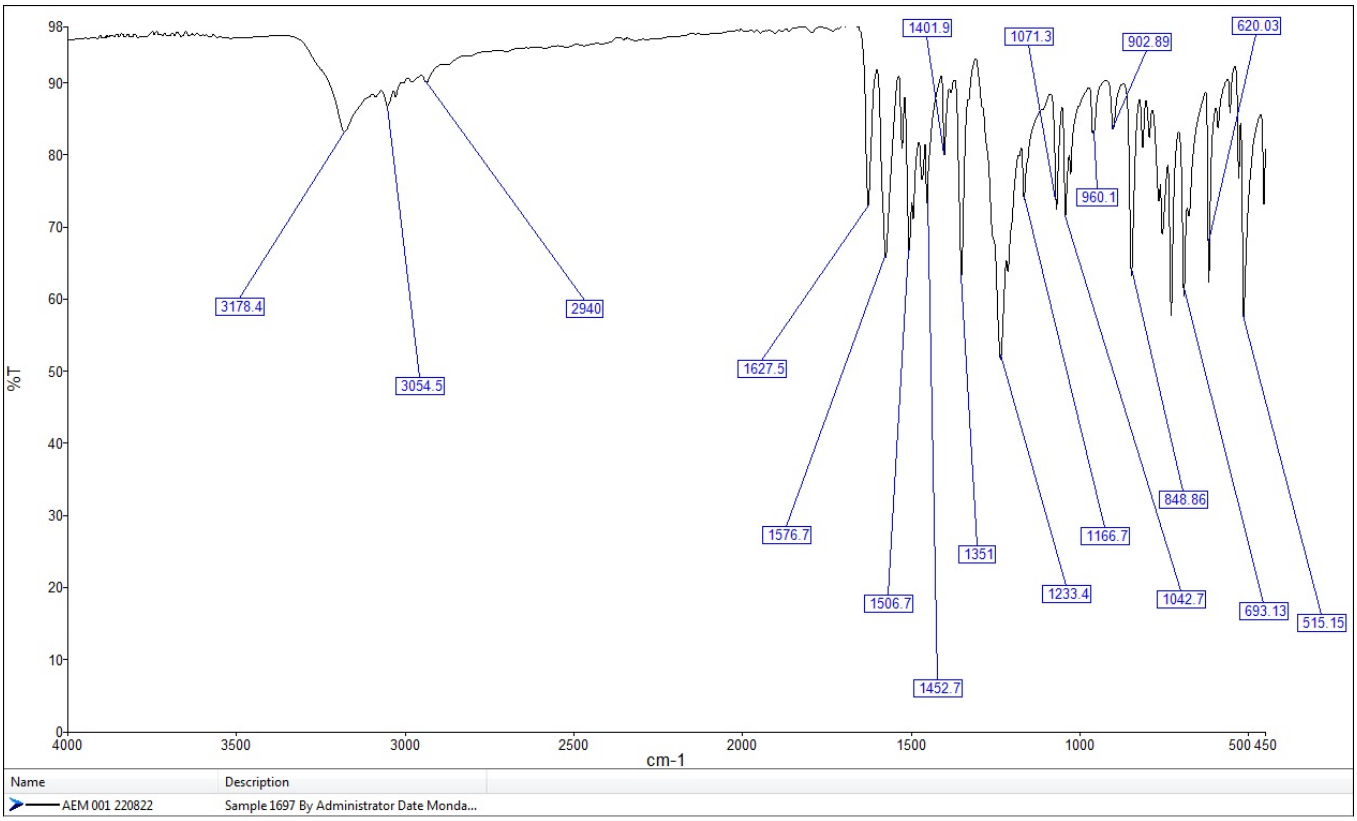

Figure S3: IR spectrum for BHM.

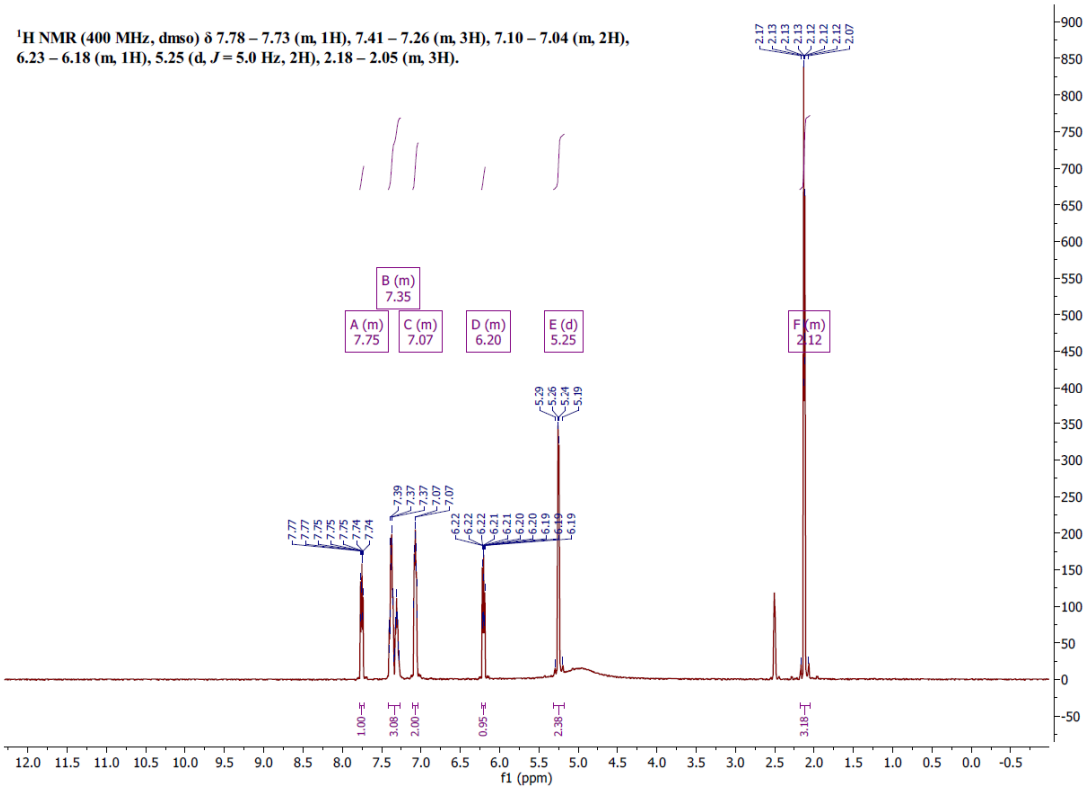

Figure S4: ^{1}H spectrum for BHM.

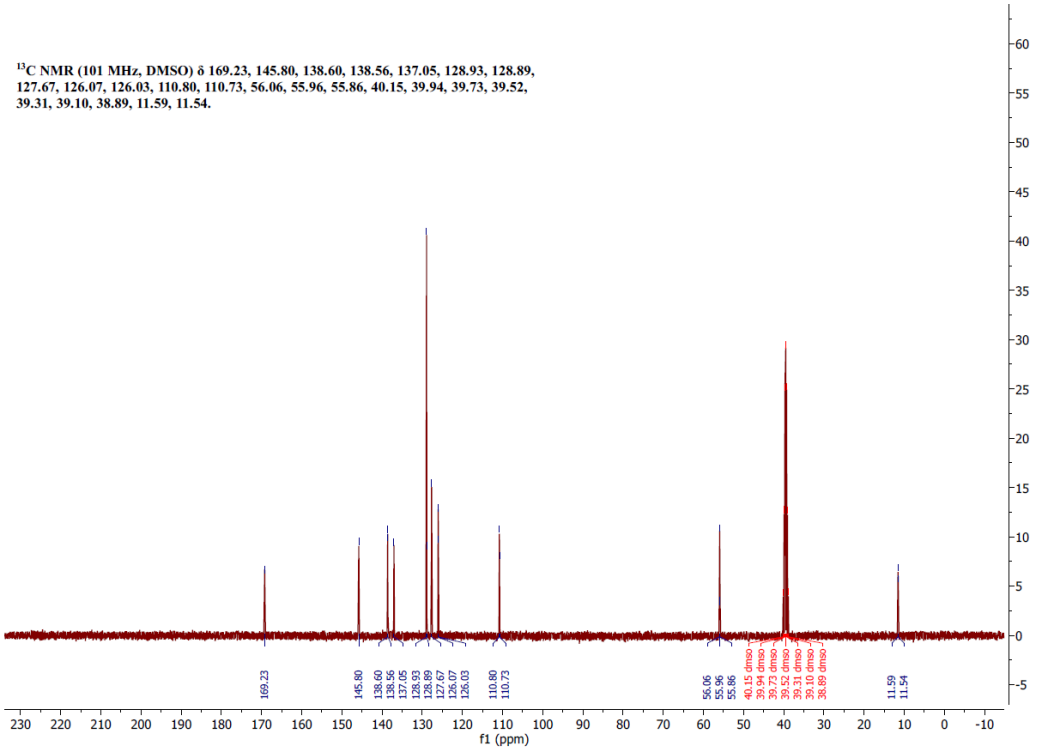

Figure S5: ^{13}C spectrum for BHM.

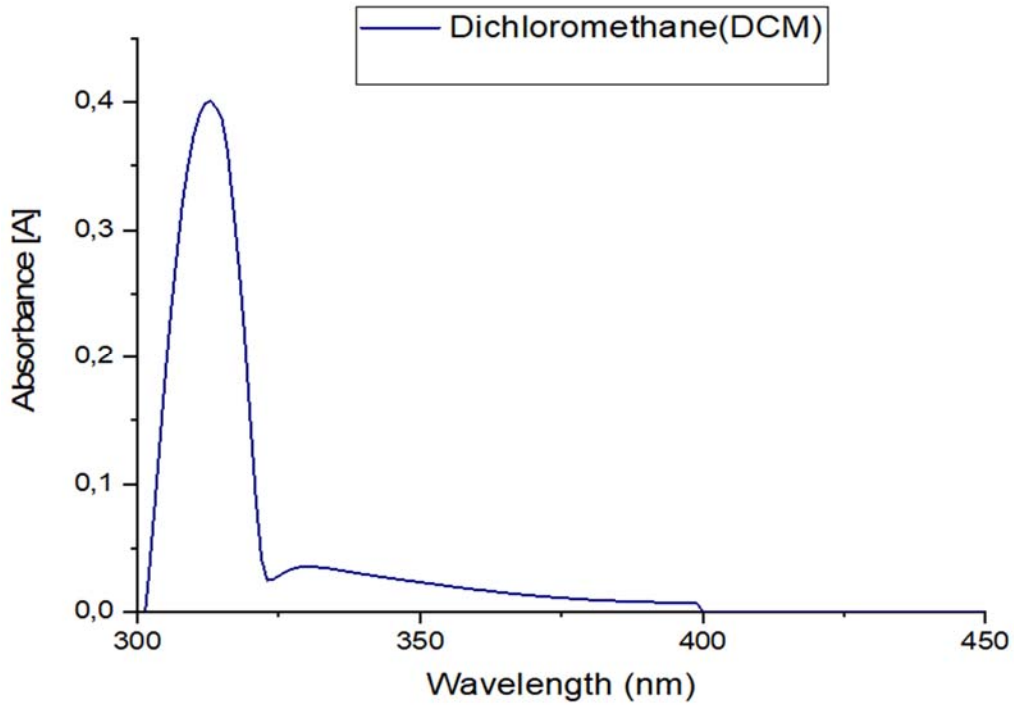

Figure S6: UV/Vis spectrum for BHM in DCM.

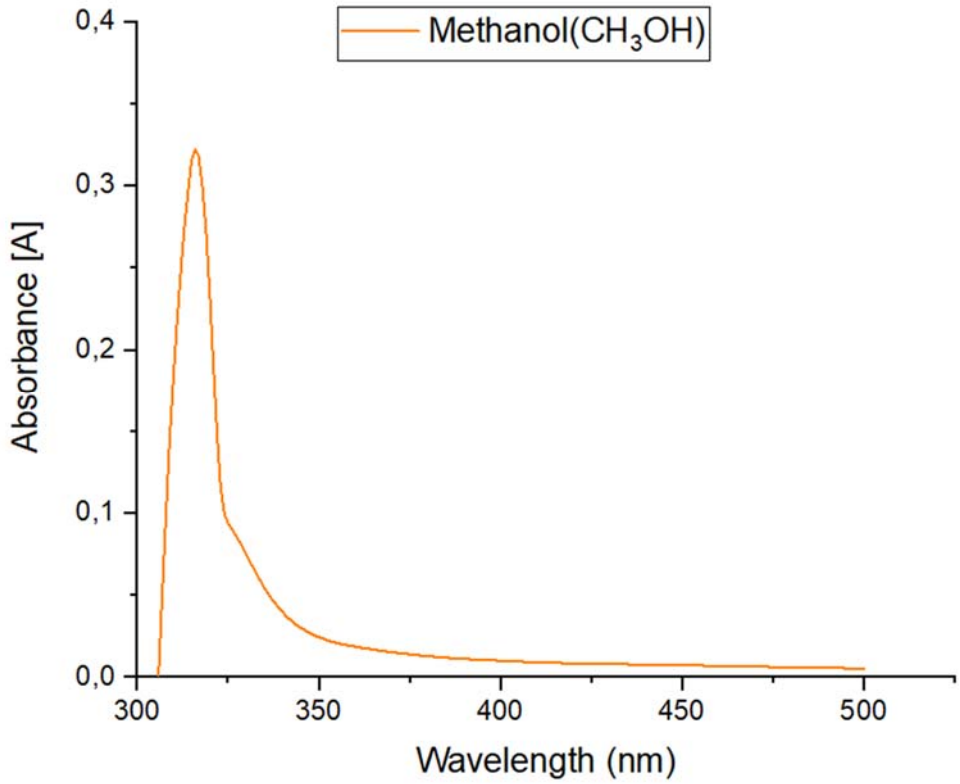

Figure S7: UV/Vis spectrum for BHM in MeOH.

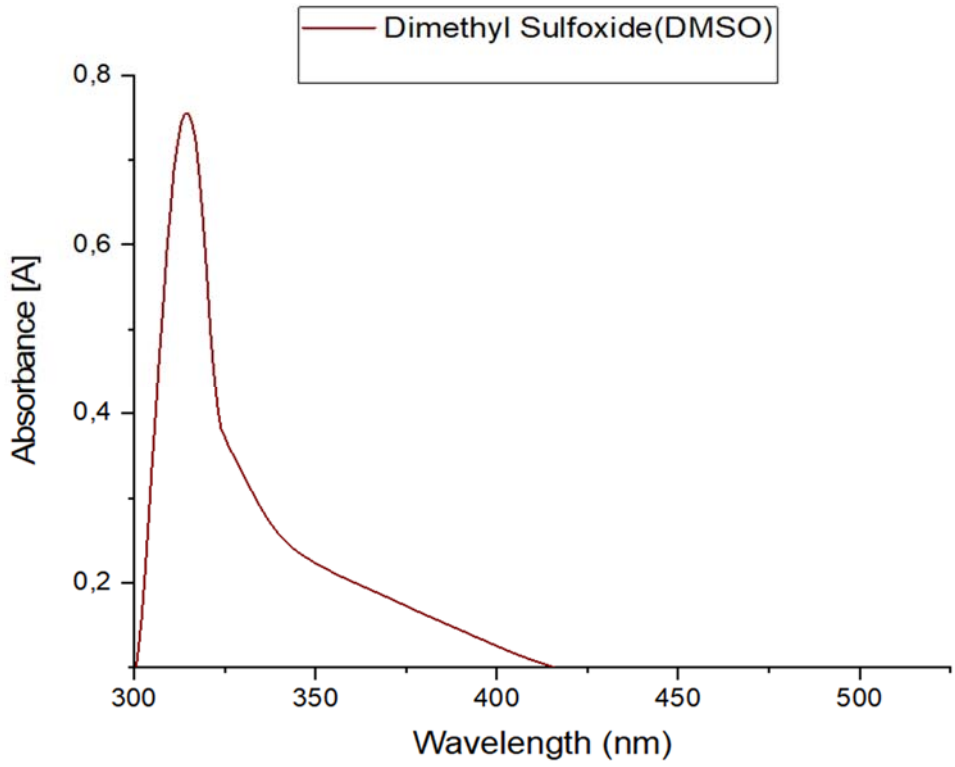

Figure S8: UV/Vis spectrum for BHM in DMSO.

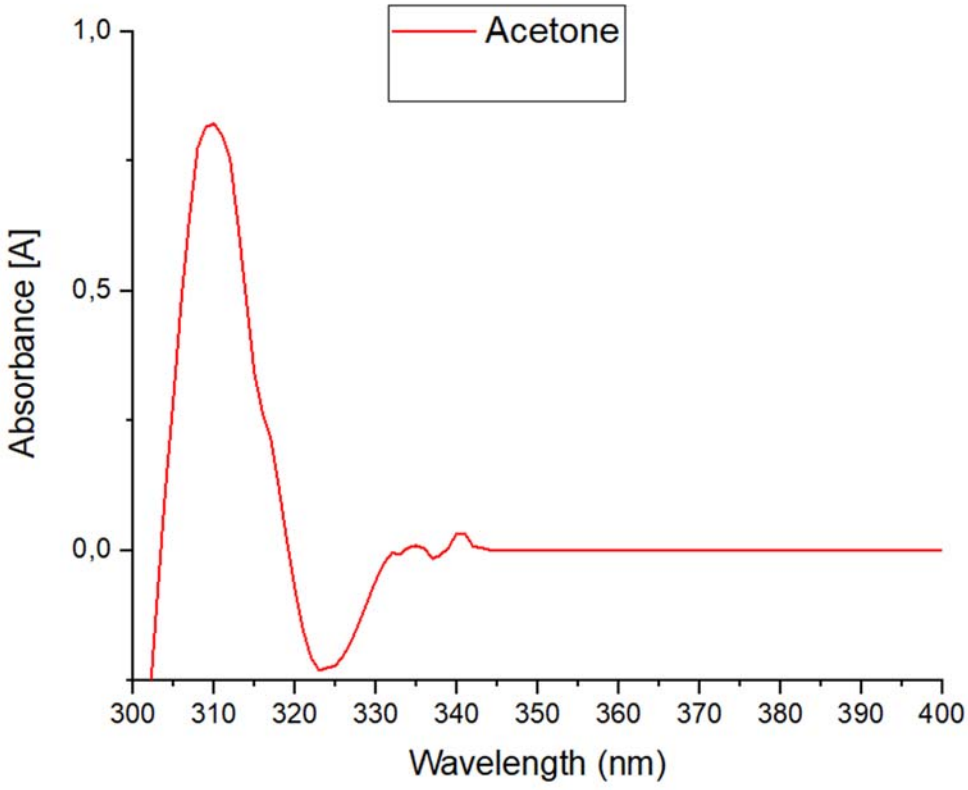

Figure S9: UV/Vis spectrum for BHM in Acetone.