Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis of an antifungal 1,2,4-triazole drug and establishment of a drug delivery system based on zeolitic imidazolate frameworks

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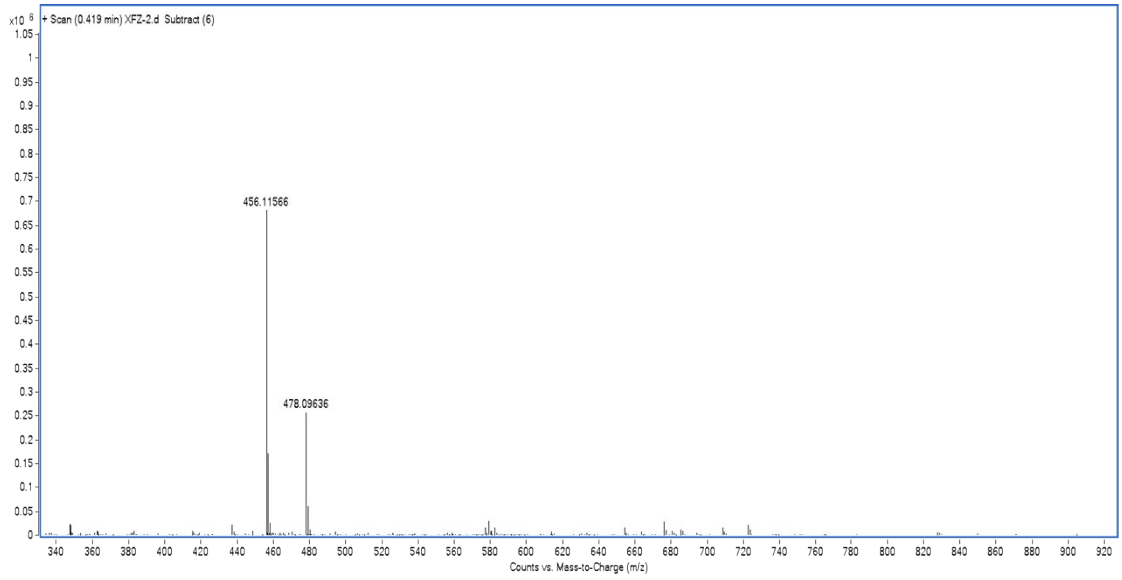

Figure 1. HRMS of TPHMB

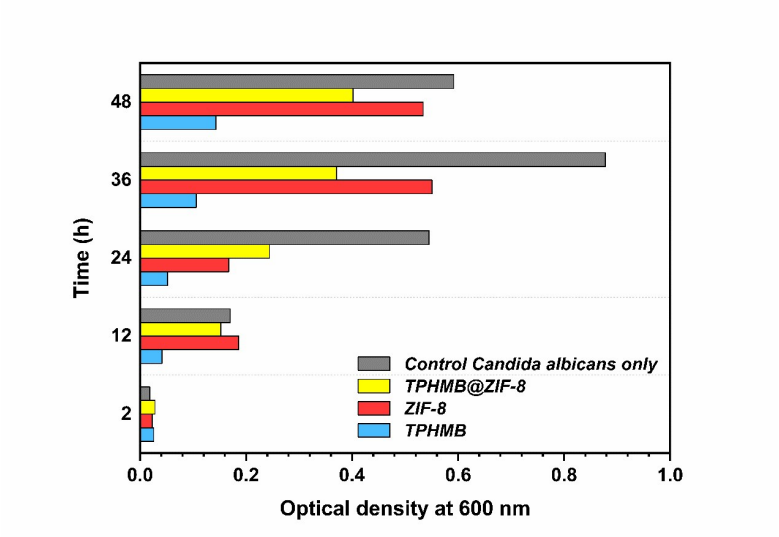

Figure 2. Assessment of the growth of Candida albicans exposed to TPHMB, ZIF-8 and TPHMB@ZIF-8

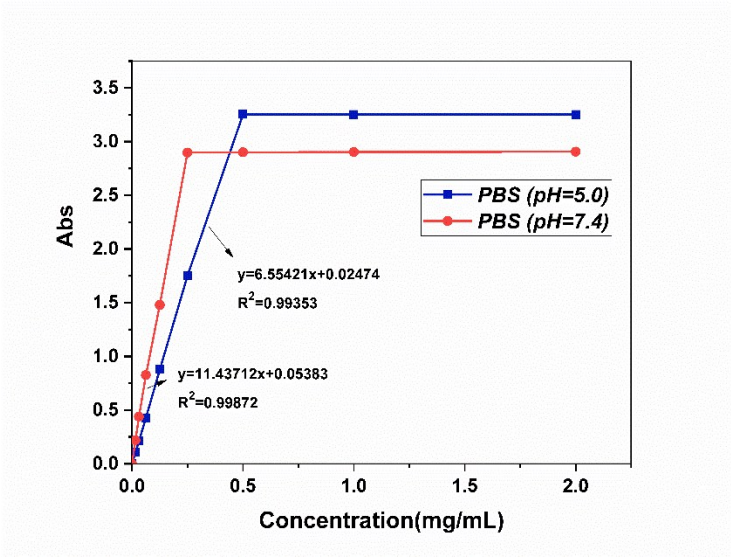

Figure 3. UV absorbance of TPHMB in PBS solution related to concentration.

Compound	TPHMB
Empirical formula	$C_{23}H_{16}F_3N_3O_4$
Formula weight	455.39
Temperature (K)	293(2)
Crystal system	Monoclinic
Space group	*P*2(1)/*c*
a (Å)	7.9040 (14)
b (Å)	29.488 (5)
c (Å)	9.471 (2)
α (°)	90
β (°)	103.898 (19)°
γ (°)	90
Volume(Å^3)	2142.9 (7)
Z	4
D_{calc} (g cm^{-3})	1.412
μ (mm^{-1})	0.12
F (000)	936
θ (°)	2.6–21.2
Reflections collected	15944
Restraints/parameters	0/301
Radiation type	Mo-Kα
F (000)	656
GOF	1.136
R [I > 2σ(I)]	R_1 = 0.1239, wR_2 = 0.3284

Table 1. Crystal data, data collection and reduction parameter of crystals of TPHMB.

bond lengths [Å]		bond angles [°]	
N3—C8	1.330 (6)	C8—N3—N1	102.7 (4)
N3—N1	1.382 (5)	C7—N2—C8	104.4 (4)
N2—C7	1.324 (6)	C7—N1—N3	109.2 (4)
N2—C8	1.359 (6)	C7—N1—C16	132.3 (4)
N1—C7	1.351 (6)	N3—N1—C16	118.4 (4)
N1—C16	1.429 (6)	N2—C7—N1	109.7 (4)
C7—C1	1.478 (7)	N2—C7—C1	122.9 (4)
C16—C17	1.371 (7)	N1—C7—C1	127.3 (4)
C16—C21	1.393 (6)	C17—C16—C21	120.6 (4)
O1—C6	1.344 (6)	C17—C16—N1	121.1 (4)
C10—C11	1.359 (7)	C21—C16—N1	118.3 (4)
C10—C9	1.387 (7)	C11—C10—C9	122.8 (5)
C14—C12	1.373 (8)	C19—C20—C21	120.3 (4)
C9—C8	1.458 (6)	C19—C20—C22	122.1 (5)
C17—C18	1.387 (7)	C21—C20—C22	117.7 (5)

C1—C2	1.382 (7)	O2—C15—C14	117.0 (5)
C1—C6	1.405 (7)	O2—C15—C9	122.8 (4)
C6—C5	1.385 (8)	C14—C15—C9	120.2 (5)
C12—C11	1.396 (8)	C12—C14—C15	120.7 (5)
C12—C13	1.451 (8)	C10—C9—C15	117.6 (4)
C2—C3	1.377 (8)	C10—C9—C8	121.3 (5)
C18—C19	1.381 (7)	C15—C9—C8	121.1 (4)
C4—C3	1.372 (9)	N3—C8—N2	113.9 (4)
C4—C5	1.369 (8)	N3—C8—C9	121.2 (4)
C20—C19	1.380 (7)	N2—C8—C9	124.8 (4)
C20—C21	1.381 (7)	C16—C17—C18	119.8 (5)
C20—C22	1.464 (8)	C2—C1—C6	118.3 (5)
C15—O2	1.356 (6)	C2—C1—C7	123.5 (4)
C15—C14	1.383 (7)	C6—C1—C7	118.1 (5)
C15—C9	1.400 (7)	C20—C21—C16	119.2 (4)
O3—C22	1.337 (7)	O1—C6—C5	115.9 (5)
O3—C23	1.450 (8)	O1—C6—C1	124.4 (5)
C22—O4	1.223 (7)	C5—C6—C1	119.6 (5)
C13—F1	1.221 (8)	C14—C12—C11	119.8 (5)
C13—F3	1.247 (10)	C14—C12—C13	119.2 (6)
C13—F2	1.264 (10)	C11—C12—C13	121.0 (6)
		C3—C2—C1	121.6 (5)
		C19—C18—C17	119.8 (5)
		C18—C19—C20	120.2 (5)
		C10—C11—C12	119.0 (5)
		C3—C4—C5	120.8 (6)
		C4—C3—C2	119.2 (6)
		C4—C5—C6	120.3 (5)
		C22—O3—C23	116.8 (6)
		O4—C22—O3	121.6 (6)
		O4—C22—C20	124.9 (6)
		O3—C22—C20	113.4 (6)
		F1—C13—F3	104.4 (9)
		F1—C13—F2	104.0 (9)
		F3—C13—F2	95.8 (8)
		F1—C13—C12	119.5 (6)
		F3—C13—C12	113.9 (8)
		F2—C13—C12	116.0 (8)

Table 2. Selected bond lengths [Å] and angles [°] for compound TPHMB at 293 K.