Supporting Information

Exploiting the potential of aryl acetamide derived Zn(II) complexes in medicinal chemistry: Synthesis, structural analysis, assessment of biological profile and molecular docking studies

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

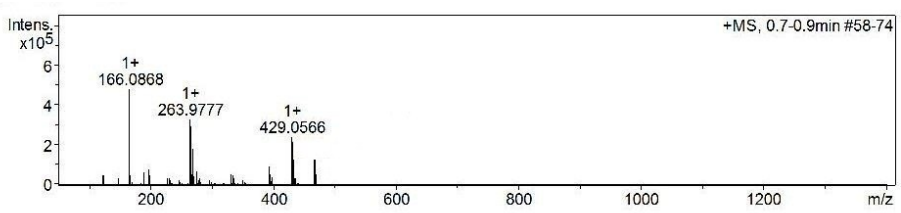
	x	y	z	U(eq)
Zn(1)	5000	11552(1)	1671(1)	20(1)
Cl(1)	5000	11532(1)	-252(1)	31(1)
Cl(2)	5000	13536(1)	2416(1)	30(1)
O(1)	4141(1)	10382(2)	2190(2)	26(1)
O(2)	2999(1)	5294(2)	-55(2)	28(1)
N(1)	3156(1)	9354(2)	3101(2)	24(1)
C(1)	3127(2)	8291(2)	2308(3)	22(1)
C(2)	3803(1)	7592(3)	2071(3)	26(1)
C(3)	3783(2)	6567(2)	1301(3)	25(1)
C(4)	3074(1)	6251(3)	761(3)	22(1)
C(5)	2383(2)	6928(3)	1025(2)	25(1)
C(6)	2413(1)	7952(2)	1797(2)	25(1)
C(7)	3695(2)	11261(3)	4010(3)	29(1)
C(8)	3678(1)	10315(2)	3031(2)	23(1)
C(9)	3700(2)	4593(3)	-376(3)	33(1)

Table S2. Bond lengths [Å] and angles [°] for **4c**.

Zn(1)-O(1)	1.9834(18)	C(3)-C(4)	1.391(4)
Zn(1)-O(1)^{i}	1.9834(18)	C(3)-H(3)	0.9500
Zn(1)-Cl(1)	2.2212(10)	C(4)-C(5)	1.394(4)
Zn(1)-Cl(2)	2.2263(9)	C(5)-C(6)	1.386(4)
O(1)-C(8)	1.248(3)	C(5)-H(5)	0.9500
O(2)-C(4)	1.373(3)	C(6)-H(6)	0.9500
O(2)-C(9)	1.436(3)	C(7)-C(8)	1.496(4)
N(1)-C(8)	1.332(3)	C(7)-H(7A)	0.9800
N(1)-C(1)	1.432(3)	C(7)-H(7B)	0.9800
N(1)-H(1)	0.791(13)	C(7)-H(7C)	0.9800
C(1)-C(2)	1.381(4)	C(9)-H(9A)	0.9800
C(1)-C(6)	1.388(4)	C(9)-H(9B)	0.9800
C(2)-C(3)	1.385(4)	C(9)-H(9C)	0.9800
C(2)-H(2)	0.9500		
O(1)-Zn(1)-O(1)^{i}	94.12(11)	C(4)-C(3)-H(3)	120.4
O(1)-Zn(1)-Cl(1)	107.23(6)	O(2)-C(4)-C(3)	123.8(2)
O(1)^{i}-Zn(1)-Cl(1)	107.23(6)	O(2)-C(4)-C(5)	115.9(2)
O(1)-Zn(1)-Cl(2)	116.52(5)	C(3)-C(4)-C(5)	120.3(2)
O(1)^{i}-Zn(1)-Cl(2)	116.52(5)	C(6)-C(5)-C(4)	119.7(2)
Cl(1)-Zn(1)-Cl(2)	113.27(4)	C(6)-C(5)-H(5)	120.2
C(8)-O(1)-Zn(1)	136.68(16)	C(4)-C(5)-H(5)	120.2
C(4)-O(2)-C(9)	117.8(2)	C(5)-C(6)-C(1)	119.9(2)
C(8)-N(1)-C(1)	123.9(2)	C(5)-C(6)-H(6)	120.1
C(8)-N(1)-H(1)	111(2)	C(1)-C(6)-H(6)	120.1
C(1)-N(1)-H(1)	125(2)	C(8)-C(7)-H(7A)	109.5
C(2)-C(1)-C(6)	120.2(2)	C(8)-C(7)-H(7B)	109.5
C(2)-C(1)-N(1)	120.0(2)	H(7A)-C(7)-H(7B)	109.5
C(6)-C(1)-N(1)	119.8(2)	C(8)-C(7)-H(7C)	109.5
C(1)-C(2)-C(3)	120.6(2)	H(7A)-C(7)-H(7C)	109.5
C(1)-C(2)-H(2)	119.7	H(7B)-C(7)-H(7C)	109.5
C(3)-C(2)-H(2)	119.7	O(1)-C(8)-N(1)	120.3(2)
C(2)-C(3)-C(4)	119.3(2)	O(1)-C(8)-C(7)	122.6(2)
C(2)-C(3)-H(3)	120.4	N(1)-C(8)-C(7)	117.1(2)

O(2)-C(9)-H(9A)	109.5	O(2)-C(9)-H(9C)	109.5
O(2)-C(9)-H(9B)	109.5	H(9A)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5	H(9B)-C(9)-H(9C)	109.5

Symmetry transformations used to generate equivalent atoms: i = -x+1,y,z



#	m/z	I %
1	124.0751	10.3
2	165.0786	13.9
3	166.0868	100.0
4	167.0894	10.6
5	188.0685	13.0
6	197.0439	16.8
7	263.9777	68.3
8	265.9747	61.1
9	266.9761	11.5
10	267.9726	37.8
11	274.0058	14.5
12	332.0148	11.3
13	334.0115	10.4
14	393.0793	19.4
15	395.0761	11.7
16	429.0566	50.0
17	430.0595	10.7
18	431.0534	44.5
19	432.0556	13.6
20	466.0557	28.2

Figure S1. Mass spectrum of complex **4c**.

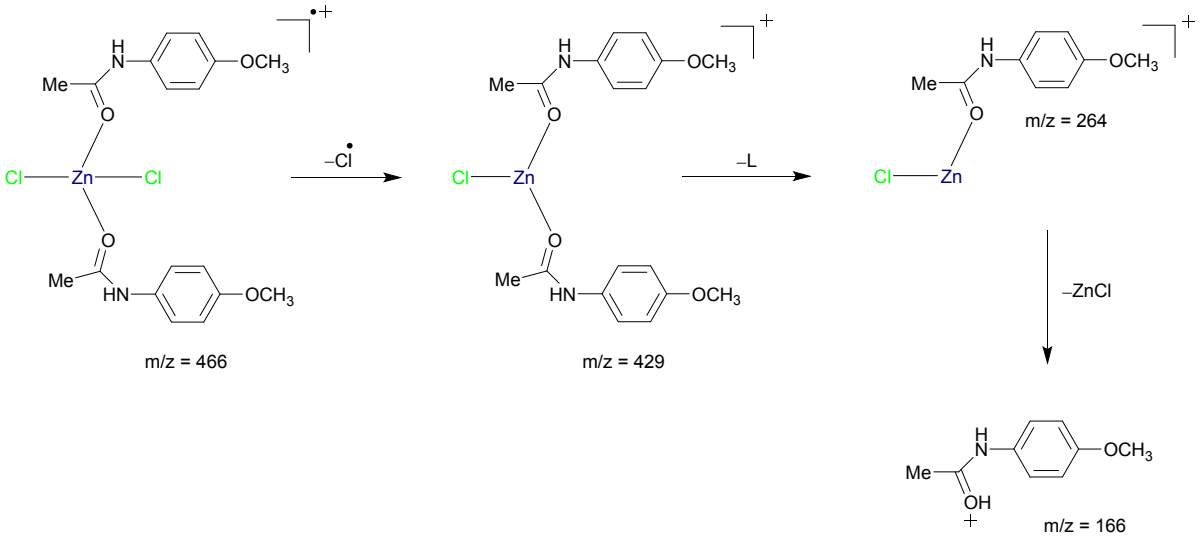


Figure S2. Proposed mass fragmentation pattern for complex **4c**.

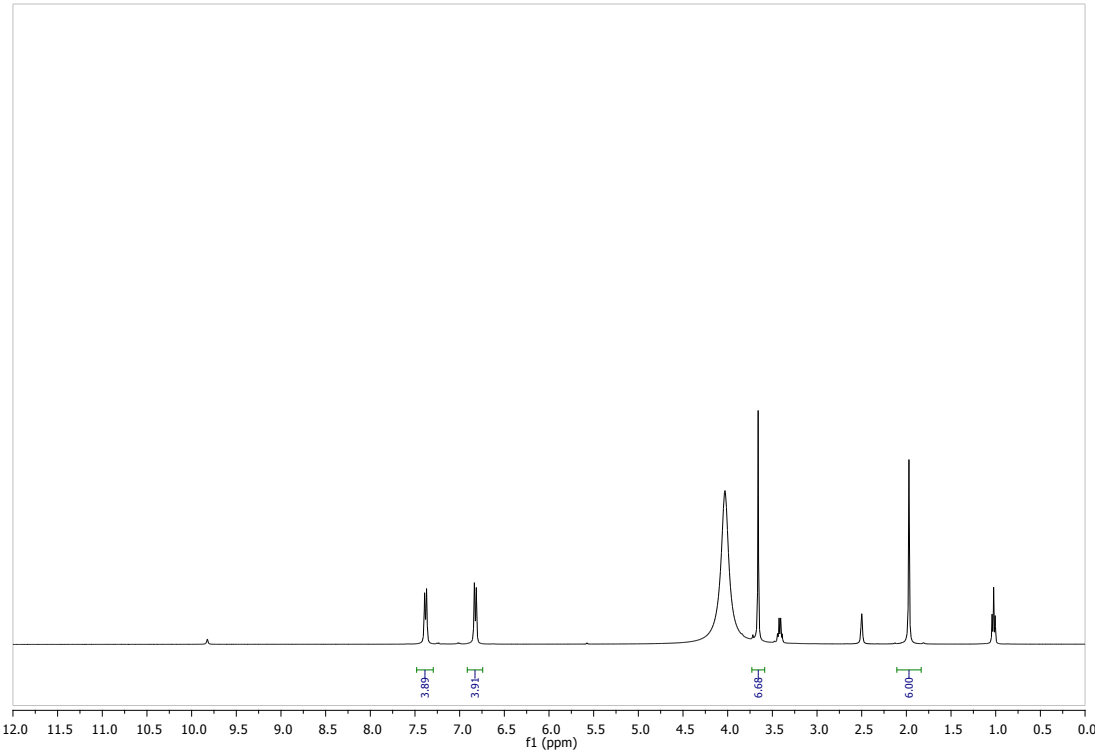


Figure S3. ^{1}H NMR spectrum of complex **4c** at room temperature (400 MHz, DMSO-d_6/D_2O).

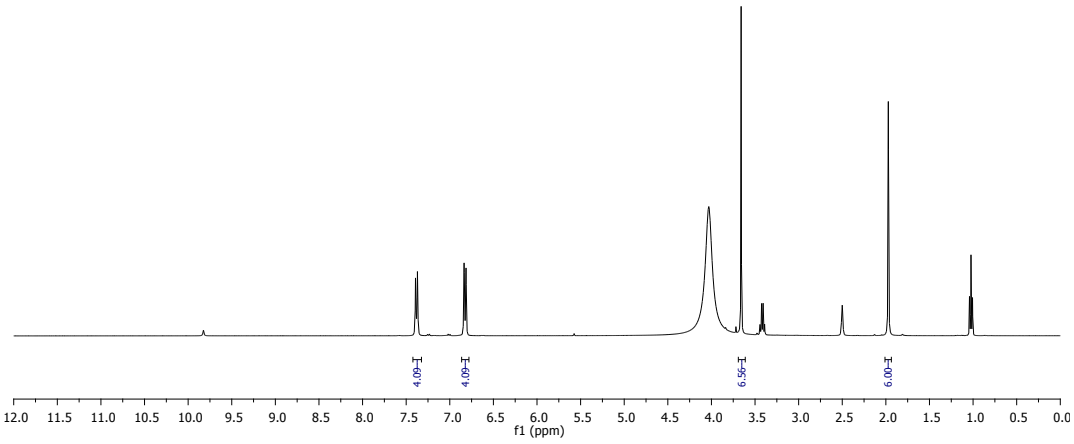


Figure S4. ^{1}H NMR spectrum of complex **4c** at room temperature after 48 h (400 MHz, DMSO-d_6/D_2O).