CHARACTERIZATION AND ANTITUMOR ACTIVITY OF FURAZANO[3,4-*g*]PTERIDINE-2,4(1*H*,3*H*)-DIONE

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Supporting information

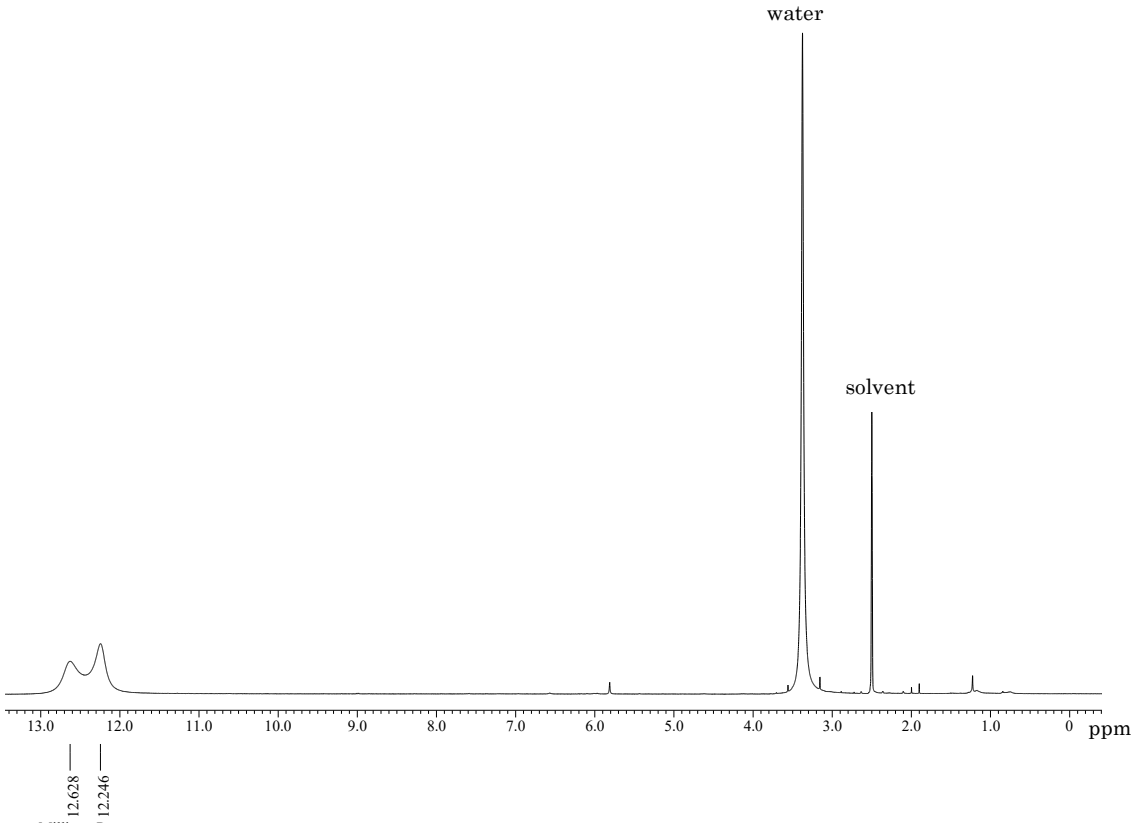

Figure S1. ^{1}H NMR spectrum of **1** (500MHz, DMSO-d_6, rt).

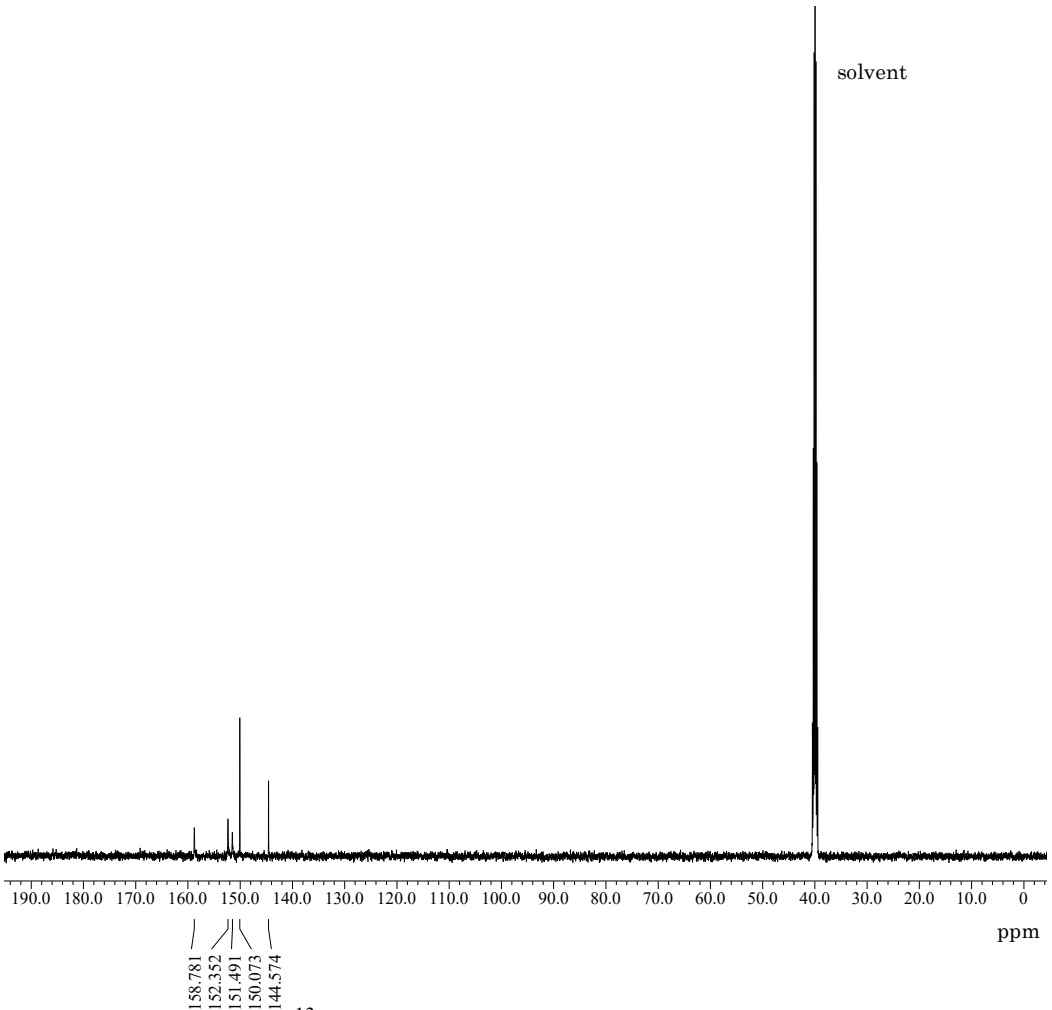

Figure S3. ^{13}C NMR spectrum of **1** (125 MHz, DMSO-d_6, rt).

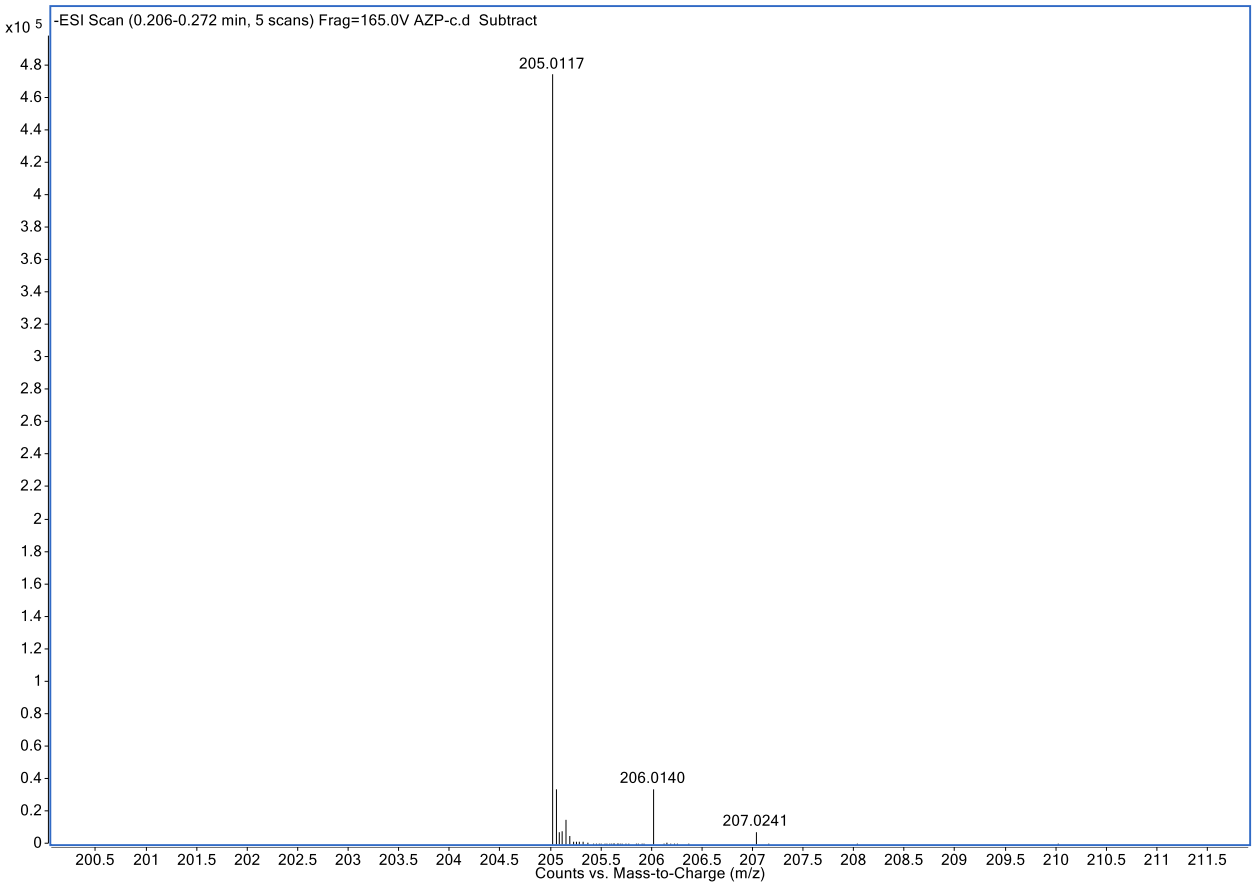

Figure S4. ESI-TOFMS spectrtrum of **1**.

Table S1. Bond lengths [Å] and angles [°] for **1**.

lengths	[Å]	angles	[°]
O(1)-C(1)	1.2193(15)	N(6)-O(3)-N(5)	113.26(9)
O(2)-C(2)	1.2198(15)	C(1)-N(1)-H(1)	118.1(10)
O(3)-N(5)	1.3960(14)	C(1)-N(1)-C(2)	126.70(11)
O(3)-N(6)	1.3741(15)	C(2)-N(1)-H(1)	115.1(10)
N(1)-H(1)	0.879(18)	C(2)-N(2)-H(2)	113.5(11)
N(1)-C(1)	1.3616(15)	C(2)-N(2)-C(3)	124.90(11)
N(1)-C(2)	1.3835(15)	C(3)-N(2)-H(2)	121.6(11)
N(2)-H(2)	0.826(17)	C(3)-N(3)-C(5)	111.82(11)
N(2)-C(2)	1.3653(16)	C(4)-N(4)-C(6)	112.23(10)
N(2)-C(3)	1.3725(16)	C(5)-N(5)-O(3)	103.52(10)
N(3)-C(3)	1.3023(16)	C(6)-N(6)-O(3)	103.51(10)
N(3)-C(5)	1.3680(16)	O(1)-C(1)-N(1)	122.41(11)
N(4)-C(4)	1.2963(15)	O(1)-C(1)-C(4)	122.48(11)
N(4)-C(6)	1.3716(16)	N(1)-C(1)-C(4)	115.10(10)
N(5)-C(5)	1.3166(16)	O(2)-C(2)-N(1)	120.97(11)
N(6)-C(6)	1.3138(16)	O(2)-C(2)-N(2)	122.00(11)
C(1)-C(4)	1.4949(17)	N(2)-C(2)-N(1)	117.04(11)
C(3)-C(4)	1.4663(17)	N(2)-C(3)-C(4)	117.35(11)
C(5)-C(6)	1.4200(17)	N(3)-C(3)-N(2)	118.23(11)
O(4)-H(4A)	0.848(14)	N(3)-C(3)-C(4)	124.43(11)
O(4)-H(4B)	0.845(14)	N(4)-C(4)-C(1)	116.72(11)
O(5)-H(5A)	0.870(14)	N(4)-C(4)-C(3)	124.39(11)
O(5)-H(5B)	0.838(14)	C(3)-C(4)-C(1)	118.89(10)
		N(3)-C(5)-C(6)	123.90(11)
		N(5)-C(5)-N(3)	126.84(12)
		N(5)-C(5)-C(6)	109.26(11)
		N(4)-C(6)-C(5)	123.23(11)
		N(6)-C(6)-N(4)	126.31(12)
		N(6)-C(6)-C(5)	110.45(11)
		H(4A)-O(4)-H(4B)	101.6(17)
		H(5A)-O(5)-H(5B)	105.6(17)