Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis, crystal structure and antiproliferative mechanisms of Gallium(III) complexes with benzoylpyridine thiosemicarbazones

Table S1 Crystal Data of Ga(III) complex (**C6**).

Table S1 Bond Lengths for C6.

Table S2 Bond Angles for C6.

^{1}H NMR Spectra for target compounds

Table S1 Crystal Data of Ga(III) complex (**C6**).

Complex name	**C6**
Empirical formula	$C_{20}H_{23}Cl_2GaN_4S$
Formula weight	492.1
Crystal system	monoclinic
Space group	$P2_1/n$
a, b, c/Å	10.6296(6), 12.6093(8), 16.8042(11)
α, β, β/°	90, 100.8541(10), 90
Volume/Å^3	2212.0(2)
Z	4
Radiation	MoKα (λ = 0.71073)

2Θ range for data collection/°	4.066 to 56.616
Index ranges	$-13 \leq h \leq 14, -16 \leq k \leq 16, -17 \leq l \leq 22$
Reflections collected	16004
Independent reflections	5481 [$R_{int} = 0.0599$, $R_{sigma} = 0.0558$]
Data/restraints/parameters	5481/0/254
Goodness-of-fit on F^2	0.949
Final R indexes [I>=2σ (I)]	$R_1 = 0.0382$, $wR_2 = 0.0969$
Final R indexes [all data]	$R_1 = 0.0571$, $wR_2 = 0.1034$
CCDC NO.	1899688

Table S2 Bond Lengths for **C6.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ga1	S1	2.3291(7)	N4	C14	1.460(3)
Ga1	Cl2	2.2070(7)	C6	C5	1.469(3)
Ga1	Cl1	2.2264(7)	C9	C10	1.387(3)
Ga1	N2	2.0581(17)	C10	C11	1.373(4)
Ga1	N1	2.098(2)	C15	C16	1.484(4)
S1	C7	1.753(2)	C15	C20	1.469(4)
N2	N3	1.350(2)	C5	C4	1.382(3)
N2	C6	1.296(3)	C4	C3	1.388(3)
N1	C5	1.354(3)	C2	C1	1.374(4)
N1	C1	1.340(3)	C2	C3	1.366(4)

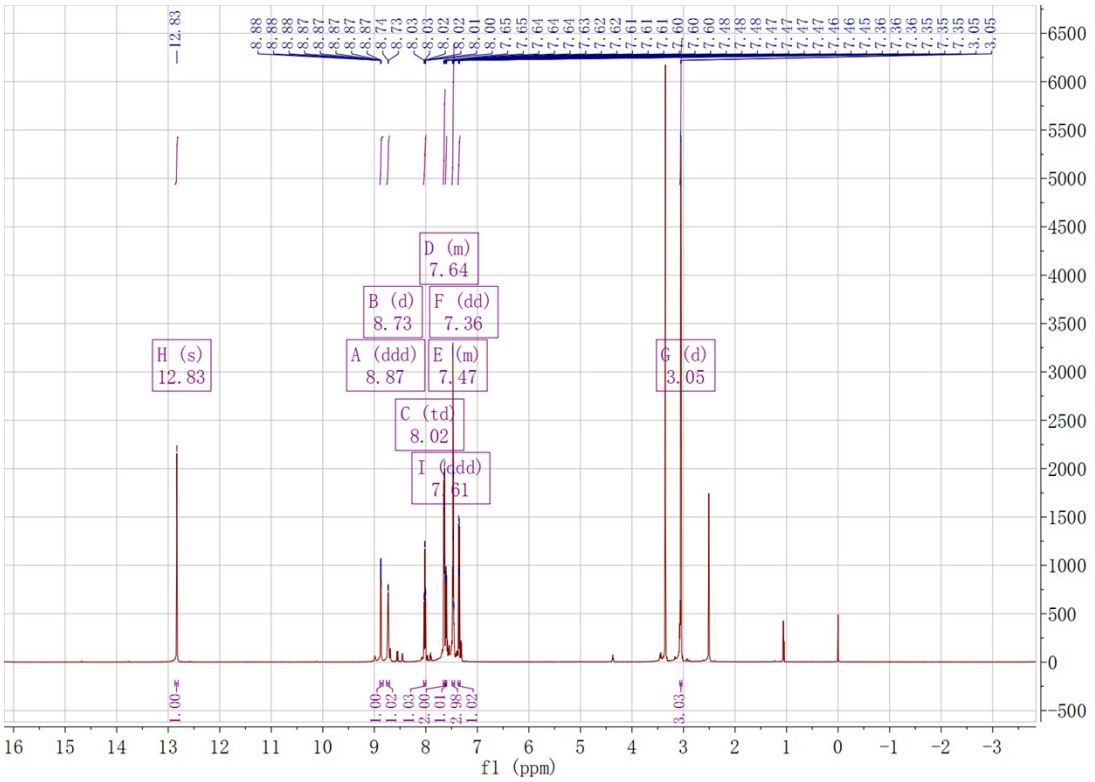
N3	C7	1.332(3)	C13	C12	1.383(3)
C7	N4	1.344(3)	C12	C11	1.368(4)
C8	C6	1.481(3)	C16	C17	1.524(6)
C8	C9	1.391(3)	C18	C19	1.454(5)
C8	C13	1.386(3)	C18	C17	1.477(6)
N4	C15	1.474(3)	C19	C20	1.521(5)

Table S3 Bond Angles for **C6**.

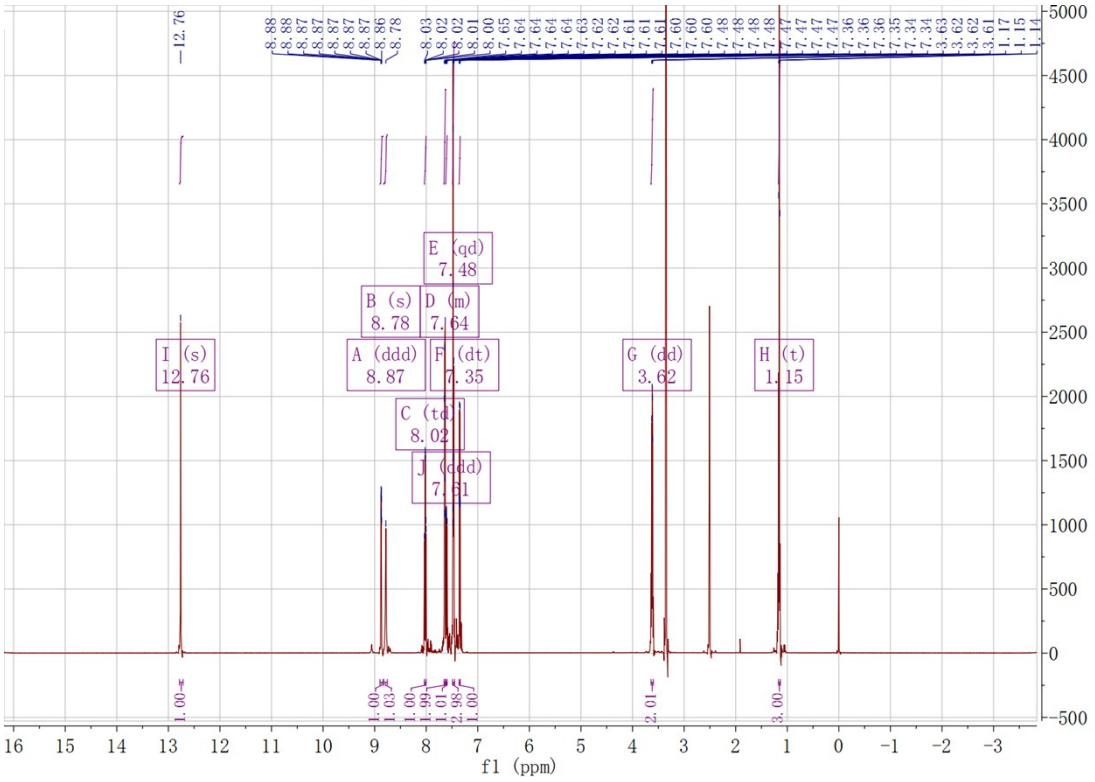
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
Cl2	Ga1	S1	107.65(3)	C7	N4	C14	121.8(2)
Cl2	Ga1	Cl1	105.34(3)	C14	N4	C15	117.9(2)
Cl1	Ga1	S1	96.81(3)	N2	C6	C8	123.68(19)
N2	Ga1	S1	80.85(5)	N2	C6	C5	113.88(19)
N2	Ga1	Cl2	99.49(6)	C5	C6	C8	122.37(19)
N2	Ga1	Cl1	154.51(6)	C10	C9	C8	120.1(2)
N2	Ga1	N1	76.42(7)	C11	C10	C9	120.3(3)
N1	Ga1	S1	147.25(5)	N4	C15	C16	111.9(3)
N1	Ga1	Cl2	99.16(6)	C20	C15	N4	113.8(2)
N1	Ga1	Cl1	93.80(6)	C20	C15	C16	110.8(3)
C7	S1	Ga1	94.21(8)	N1	C5	C6	115.23(19)
N3	N2	Ga1	120.51(13)	N1	C5	C4	121.1(2)
C6	N2	Ga1	119.31(14)	C4	C5	C6	123.7(2)
C6	N2	N3	119.78(17)	C5	C4	C3	119.2(2)

C5	N1	Ga1	114.83(14)	C3	C2	C1	119.2(2)
C1	N1	Ga1	126.31(17)	C12	C13	C8	120.4(2)
C1	N1	C5	118.8(2)	N1	C1	C2	122.5(2)
C7	N3	N2	113.33(18)	C11	C12	C13	120.3(2)
N3	C7	S1	123.86(17)	C12	C11	C10	120.1(2)
N3	C7	N4	116.3(2)	C2	C3	C4	119.3(3)
N4	C7	S1	119.86(17)	C15	C16	C17	110.1(4)
C9	C8	C6	119.4(2)	C19	C18	C17	110.9(3)
C13	C8	C6	121.7(2)	C18	C19	C20	112.1(4)
C13	C8	C9	118.9(2)	C15	C20	C19	111.4(3)
C7	N4	C15	119.95(19)	C18	C17	C16	112.9(5)

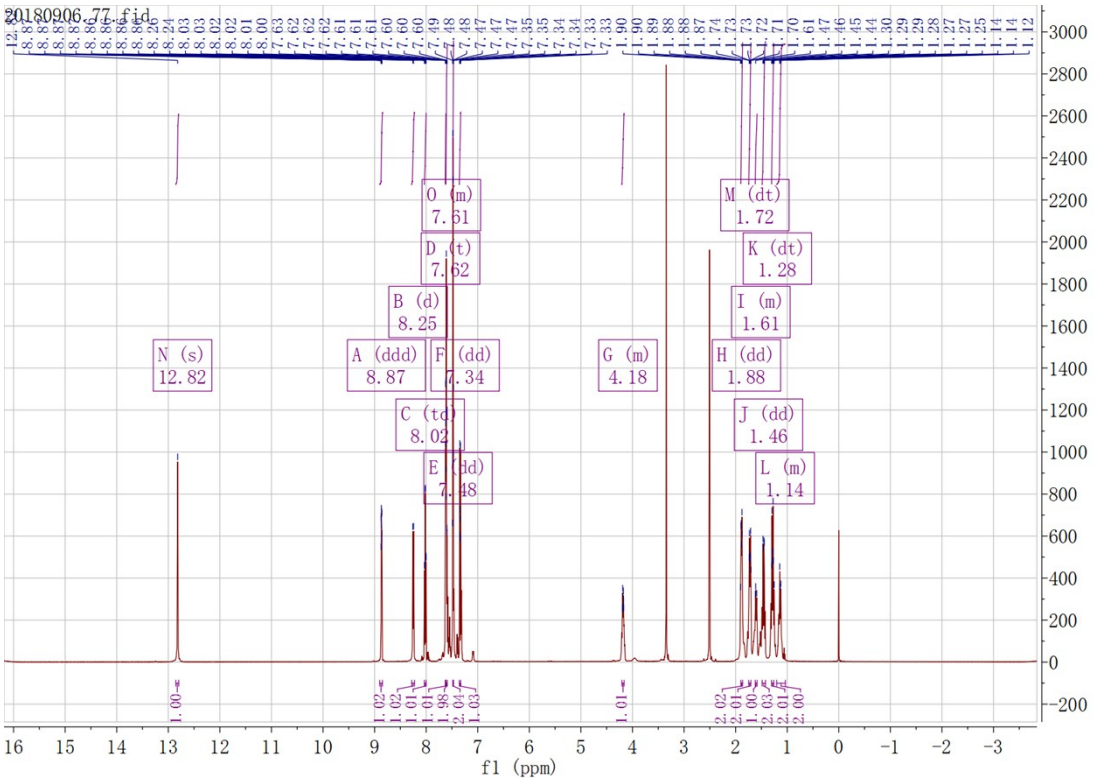
^{1}H NMR Spectra and HRMS for target compounds



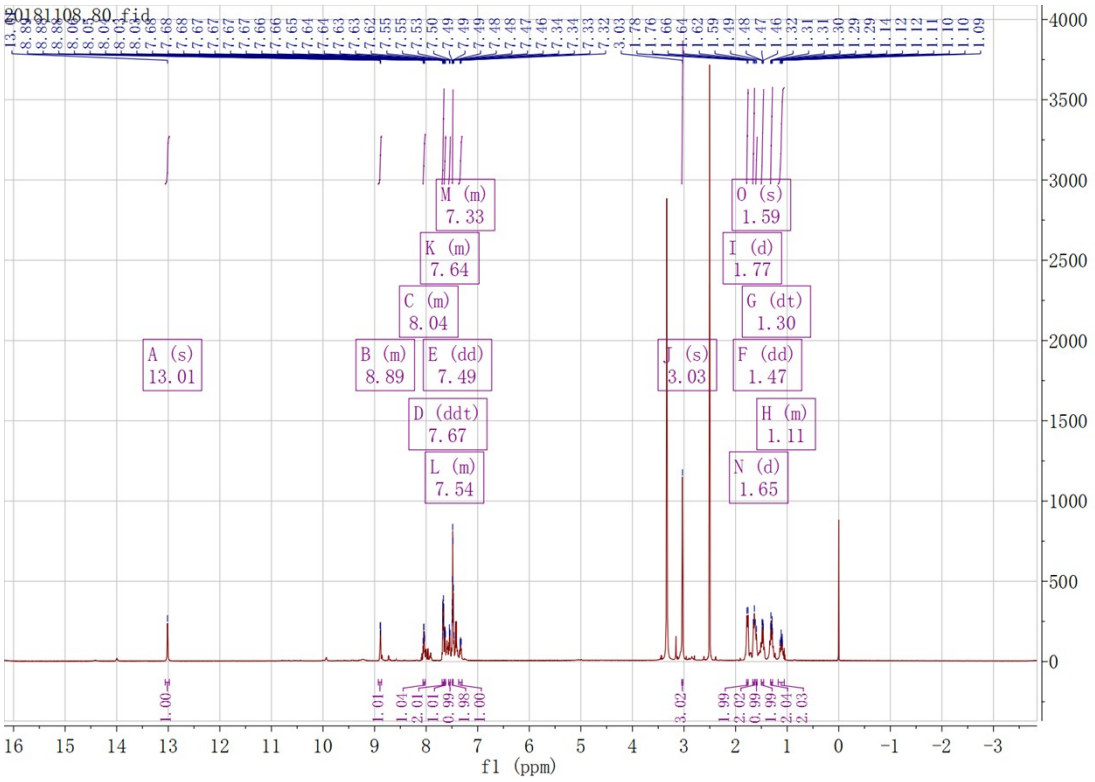
^{1}H NMR Spectra for L2



^{1}H NMR Spectra for L3



^{1}H NMR Spectra for L4



^{1}H NMR Spectra for L6