Supporting Information

Titanium isopropoxide complexes supported by pyrrolyl Schiff base ligands: syntheses, structures, and antitumor activity

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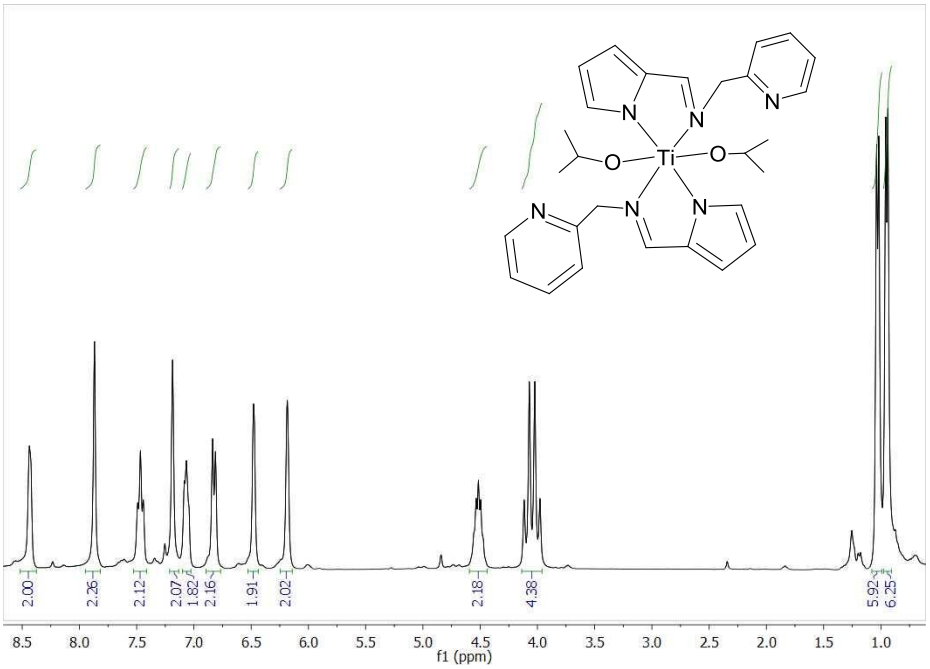
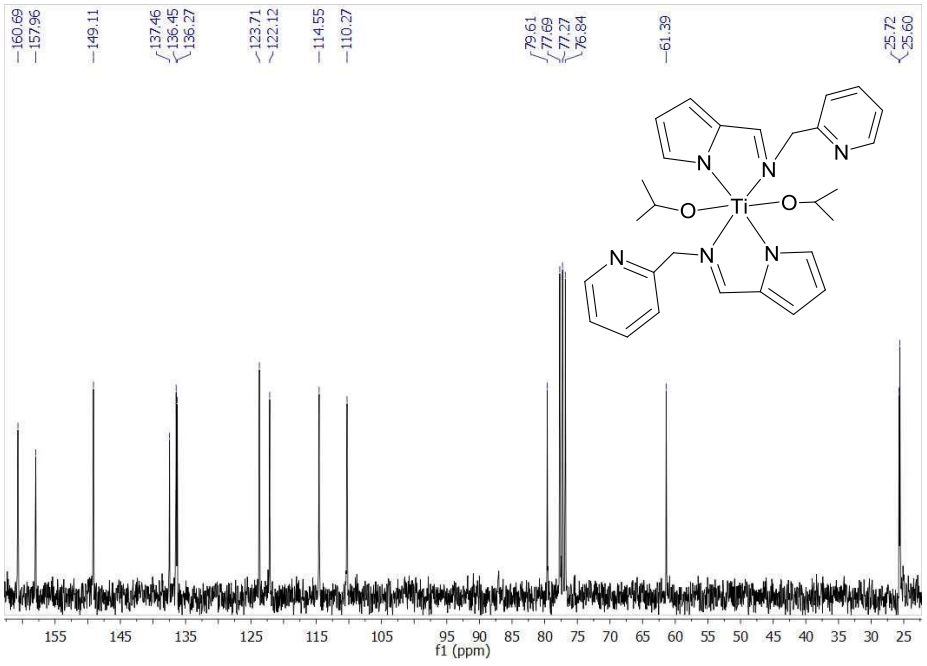
1. ^{1}H and ^{13}C NMR spectra for the complexes **1**-**4**.
2. Crystallography data for complexes **1** and **3**.

1. ^{1}H and ^{13}C NMR spectra for the complexes **1-4**.

1.1 ^{1}H and ^{13}C NMR spectra for $Ti(O^{i}Pr)_2(L1)_2$ (**1**)

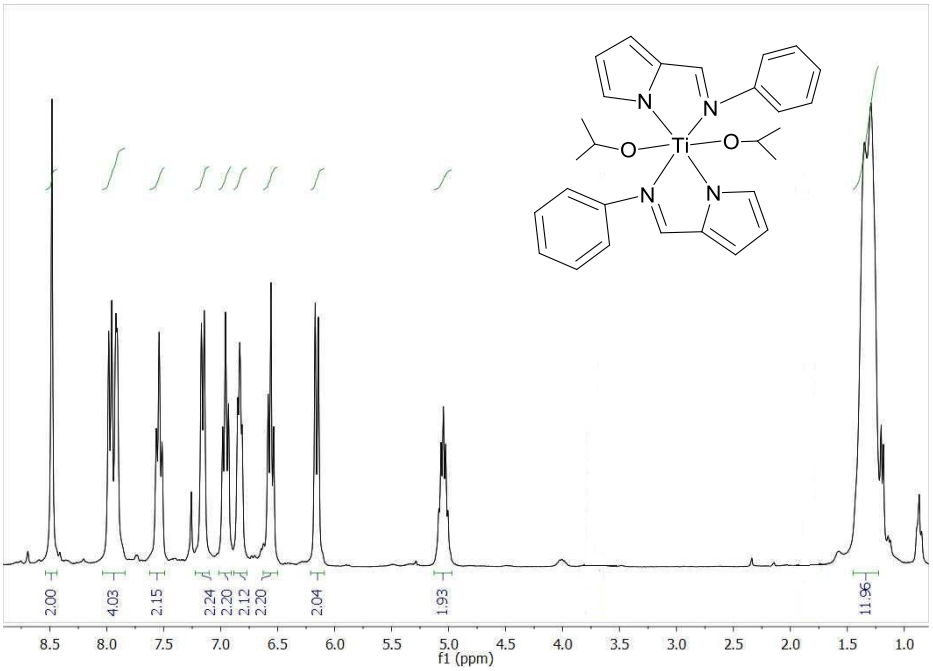
^{1}H NMR (300 MHz,$CDCl_3$) δ 8.44 (s, 2H, N=CH), 7.87 (s, 2H, pyridine-H), 7.47 (t, 2H, pyridine-H), 7.19 (s, 2H, pyridine-H), 7.07 (d, 2H, pyridine-H), 6.82 (d, 2H, pyrrole-H), 6.48 (s, 2H, pyrrole-H), 6.18 (s, 2H, pyrrole-H), 4.59–4.44 (m, 2H, OCH), 4.05 (q, 4H, NCH2), 1.03 (d, 6H, CH3), 0.95 (d, 6H, CH3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.69, 157.96, 149.11, 137.46, 136.45, 136.27, 123.71, 122.12, 114.55, 110.27, 79.61, 61.39, 25.72, 25.60.

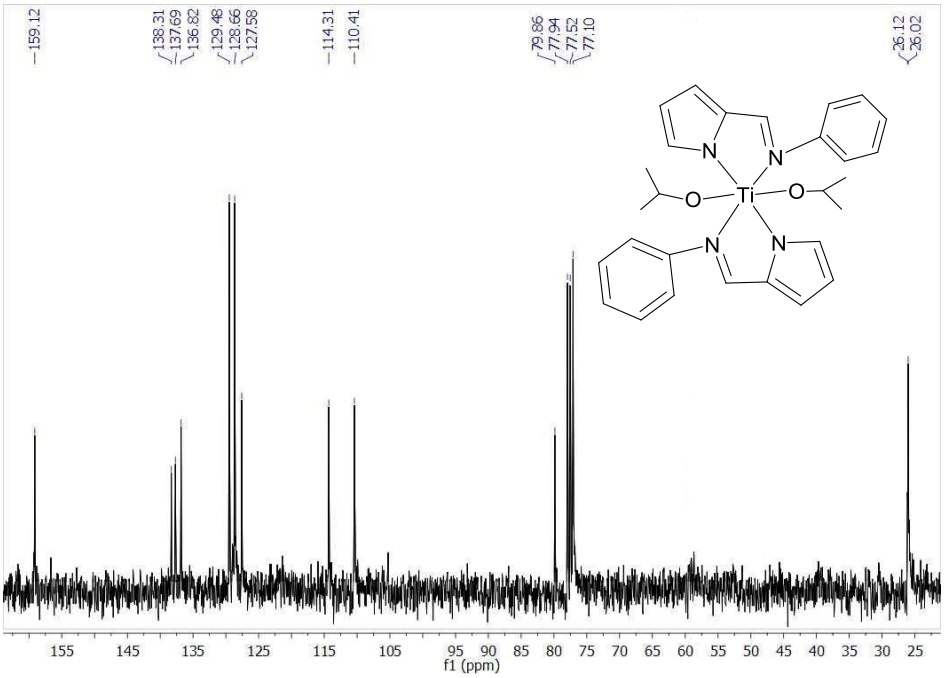




1.2 ^{1}H and ^{13}C NMR spectra for Ti($O^{i}Pr$)$_2$(L2)$_2$ (**2**)

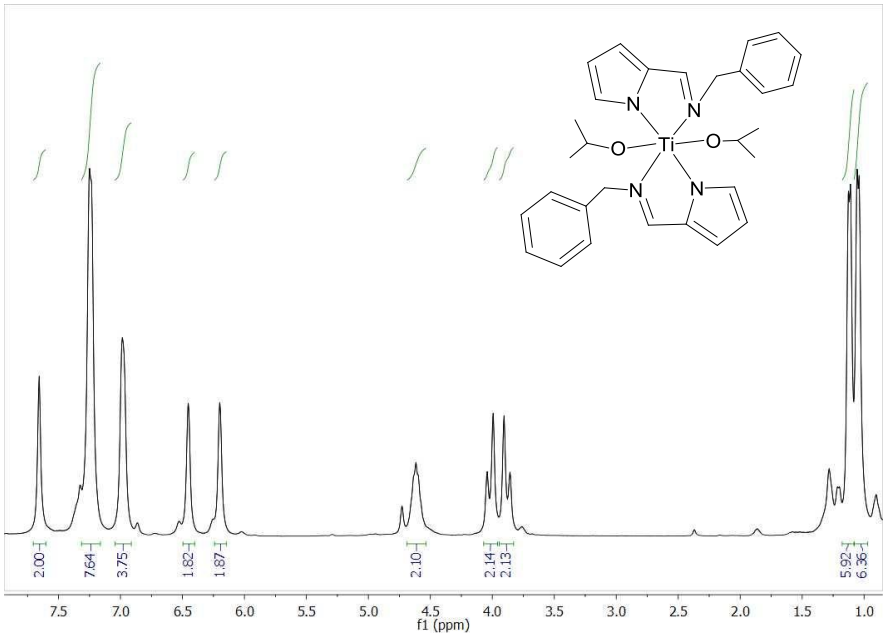
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 (s, 2H, N=CH), 7.94 (s, 4H, Ar-H), 7.54 (s, 2H, Ar-H), 7.16 (s, 2H, Ar-H), 6.96 (s, 2H, Ar-H), 6.89 (m, 2H, pyrrole-H), 6.56 (t, 2H, pyrrole-H), 6.16 (d, 2H, pyrrole-H), 5.05 (t, 2H, OCH), 1.32 (d, 12H, CH_3). **^{13}C** NMR (75 MHz, $CDCl_3$) δ 159.12, 138.31, 137.69, 136.82, 129.48, 128.66, 127.58, 114.31, 110.41, 79.86, 26.12, 26.02.

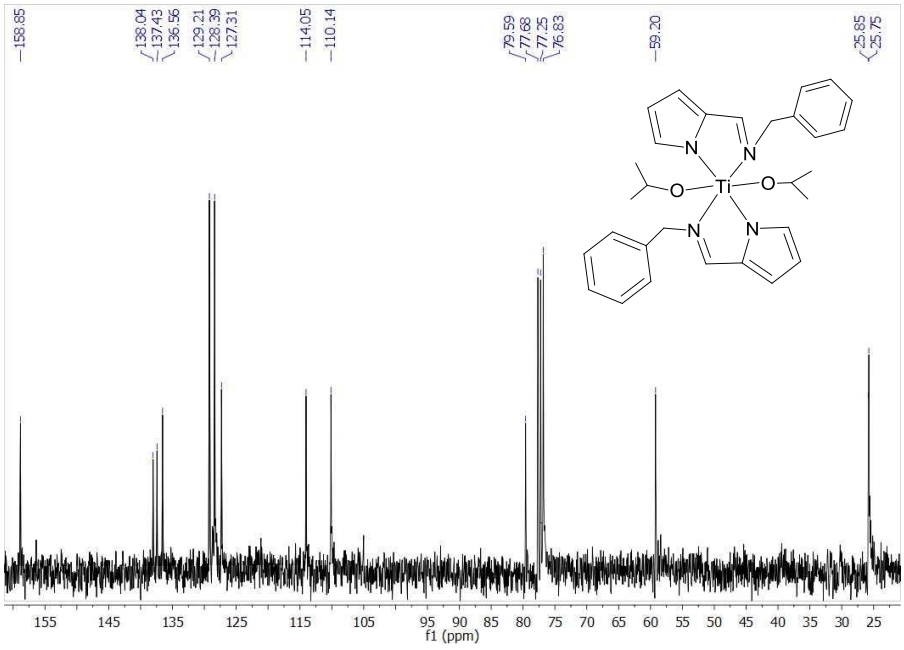




1.3 ^{1}H and ^{13}C NMR spectra for Ti($O^{i}Pr$)$_2$(L3)$_2$ (**3**)

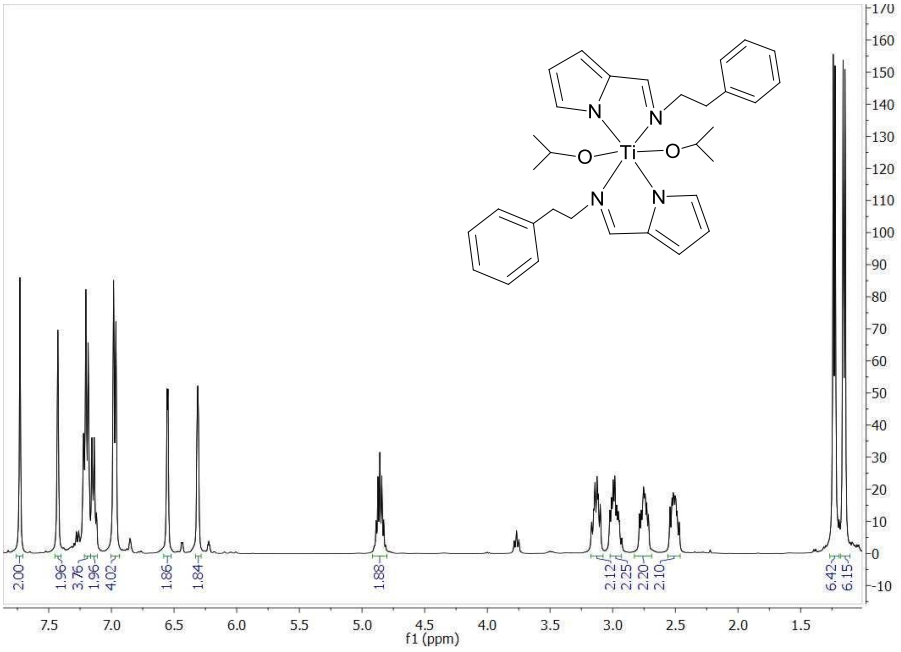
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (s, 2H, N=CH), 7.45 (s, 8H, Ar-H), 7.18 (s, 4H, Ar-H+pyrrole-H), 6.65 (s, 2H, pyrrole-H), 6.40 (s,2H, pyrrole-H), 4.82 (s, 2H, OCH), 4.22 (d, 2H, NCH_2), 4.08 (d, 2H, NCH_2), 1.38–1.28 (m, 6H, CH_3), 1.25 (d, 6H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.85, 138.04, 137.43, 136.56, 129.21, 128.39, 127.31, 114.05, 110.14, 79.59, 59.20, 25.85, 25.75.

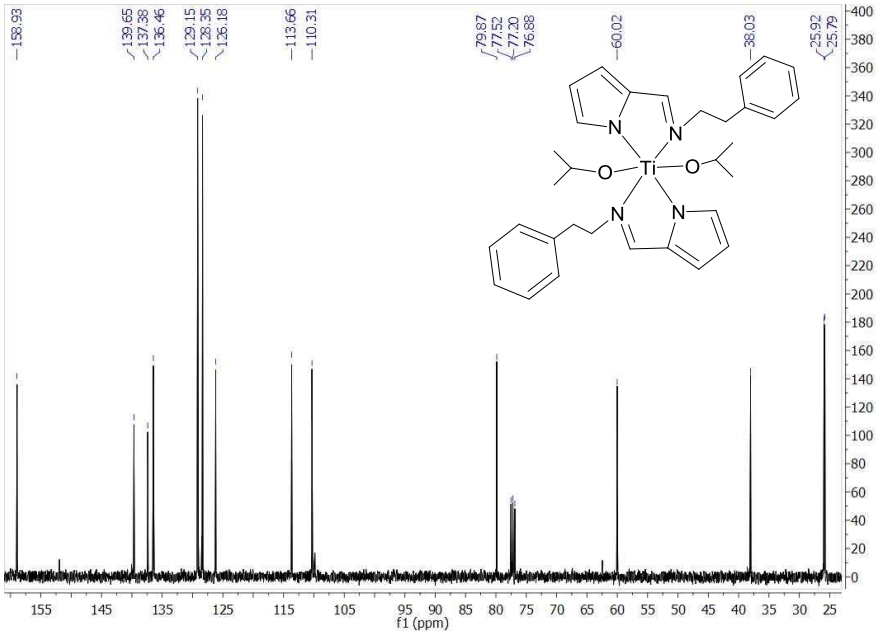




1.4 ^{1}H and ^{13}C NMR spectra for Ti($O^{i}Pr$)$_2$(L4)$_2$ (**4**)

^{1}H NMR (400 MHz,$CDCl_3$) δ 7.73 (s, 2H, N=CH), 7.43 (s, 2H, Ar-H), 7.19 (d, 4H, Ar-H), 7.17–7.11 (m, 2H, Ar-H), 6.97 (d, 4H, Ar-H+ pyrrole-H), 6.55 (d, 2H, pyrrole-H), 6.31 (d, 2H, pyrrole-H), 4.92–4.80 (m, 2H, OCH), 3.13 (td, 2H , CH_2-pyridine), 3.02–2.93 (m, 2H, CH_2-pyridine), 2.83–2.69 (m, 2H, NCH_2), 2.56–2.46 (m, 2H, NCH_2), 1.22 (t, 6H, CH_3), 1.15 (d, 6H, CH_3). ^{13}C NMR (101MHz, $CDCl_3$) δ 158.93, 139.65, 137.38, 136.46, 129.15, 128.35, 126.18, 113.66, 110.31, 79.87, 60.02, 38.03, 25.92, 25.79.





2. Crystallography data for complexes **1** and **3**

2.1 Crystal data for **1** and **3**

Table S1 Crystal data and structure refinements for **1** and **3**

	1	**3**
Formula [a]	$C_{28}H_{34}N_6O_2Ti$	$C_{30}H_{36}N_4O_2Ti$
M / g·mol^{-1} [a]	534.51	532.53
T/K	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	P21/c	P21/c
a / Å	10.2191(8)	10.268(2)
b / Å	11.4180(10)	11.468(3)
c / Å	24.491(2)	24.648(6)
α /°	90.00	90.00
β /°	100.554(2)	100.635(4)
γ /°	90.00	90.00
V / Å^3	2809.3(4)	2852.6(11)
Z	4	4
ρ_c /g·cm^{-3}	1.264	1.240
μ / mm^{-1}	0.340	0.332
F(000)	1128.0	1128.0
θ range/°	3.94 to 54.24°	3.36 to 50°
Measd/ independent	6183	5014
R_{int} reflections	0.0258	0.0538
obsd reflns [$I > 2\sigma$ (I)]	6183/4/330	5014/24/338
GOF on F^2	1.026	1.109
R_1 [c]	0.0668	0.0894
wR_2 [d,e]	0.1906	0.2362
$(\Delta\rho)_{max,min}$/e·Å^{-3}	1.27/-1.17	1.29/-0.56

[a] Including solvent molecules. [b] Mo Kα radiation. [c] $R_1 = \Sigma(||F_o|-|F_c||)/\Sigma(|F_o|)$ for observed reflections. [d] $w=1/[\sigma^2(F_o^2)+(\alpha P)^2+bP]$ and $P = [\max(F_o^2,0)+2F_c^2]/3$. [e] $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ for all data.

2.2 Bond angles and distances for complexes **1** and **3**

Table S2 Selected bond lengths (Å) and angles (°) for **1** and **3**

1			
Ti(1)-O(2)	1.761(2)	Ti(1)-N(1)	2.106(2)
Ti(1)-O(1)	1.783(2)	Ti(1)-N(5)	2.255(2)
Ti(1)-N(4)	2.094(2)	Ti(1)-N(2)	2.293(2)
O(2)-Ti(1)-O(1)	101.42(10)	N(4)-Ti(1)-N(5)	74.38(9)
O(2)-Ti(1)-N(4)	95.06(10)	N(1)-Ti(1)-N(5)	86.43(8)
O(1)-Ti(1)-N(4)	101.54(9)	O(2)-Ti(1)-N(2)	91.38(9)
O(2)-Ti(1)-N(1)	100.58(9)	O(1)-Ti(1)-N(2)	164.15(9)
O(1)-Ti(1)-N(1)	94.27(9)	N(4)-Ti(1)-N(2)	86.44(8)
N(4)-Ti(1)-N(1)	155.09(9)	N(1)-Ti(1)-N(2)	74.00(8)
O(2)-Ti(1)-N(5)	165.49(9)	N(5)-Ti(1)-N(2)	78.25(8)
O(1)-Ti(1)-N(5)	90.61(9)		
3			
Ti(1)-O(2)	1.764(3)	Ti(1)-N(1)	2.109(4)
Ti(1)-O(1)	1.787(3)	Ti(1)-N(4)	2.264(4)
Ti(1)-N(3)	2.103(4)	Ti(1)-N(2)	2.304(4)
O(2)-Ti(1)-O(1)	101.50(18)	N(3)-Ti(1)-N(4)	74.27(14)
O(2)-Ti(1)-N(3)	95.35(16)	N(1)-Ti(1)-N(4)	86.24(15)
O(1)-Ti(1)-N(3)	101.51(16)	O(2)-Ti(1)-N(2)	91.37(16)
O(2)-Ti(1)-N(1)	100.58(16)	O(1)-Ti(1)-N(2)	164.19(15)
O(1)-Ti(1)-N(1)	94.32(16)	N(3)-Ti(1)-N(2)	86.21(14)
N(3)-Ti(1)-N(1)	154.82(16)	N(1)-Ti(1)-N(2)	74.11(14)
O(2)-Ti(1)-N(4)	165.64(16)	N(4)-Ti(1)-N(2)	78.26(14)
O(1)-Ti(1)-N(4)	90.47(15)		