

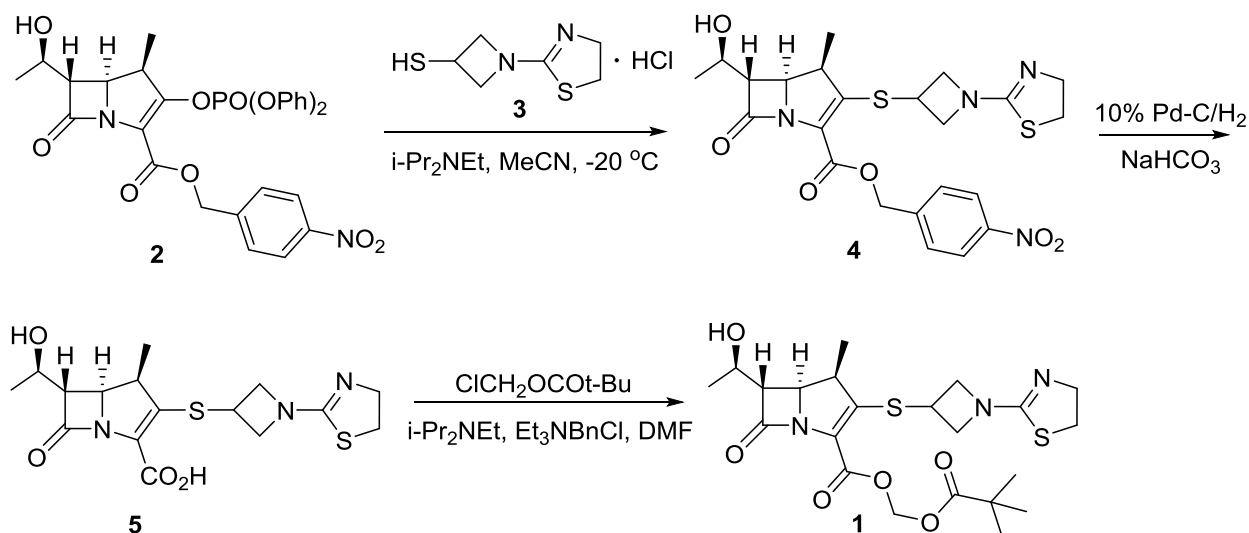
# Supporting Information

## Crystal Structure of Tebipenem Pivoxil

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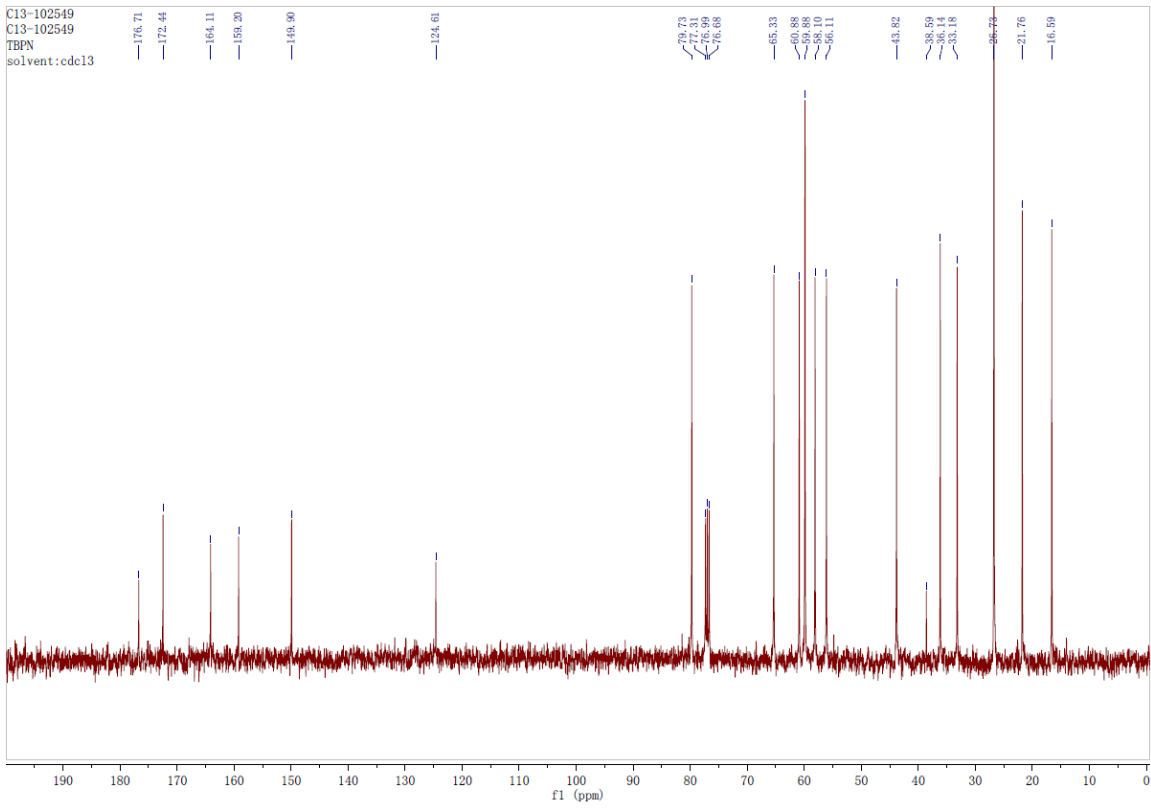
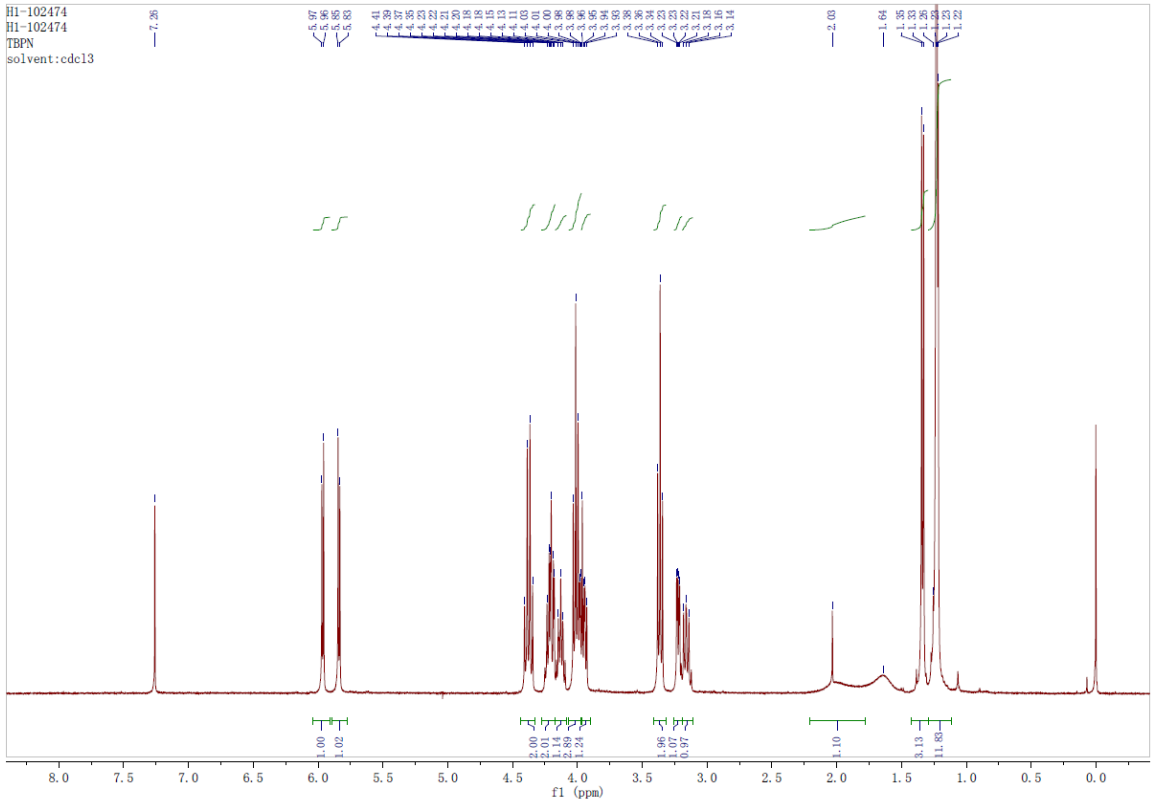
### 1. Synthesis and characterization of tebipenem pivoxil.

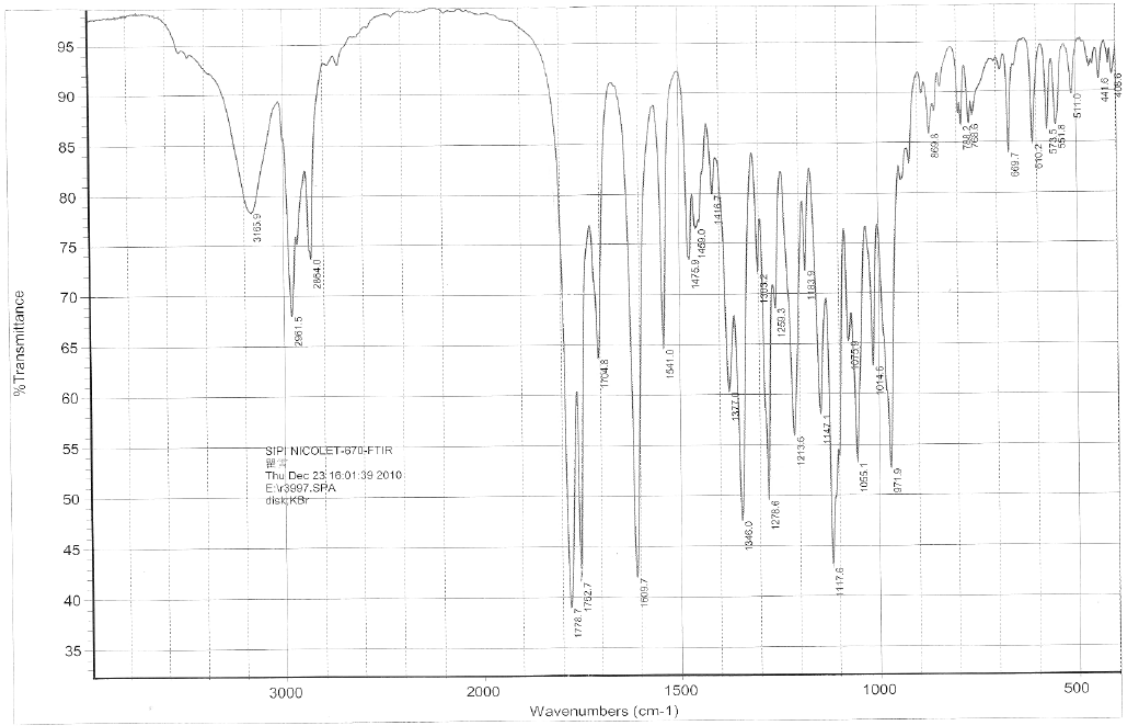


**Table S1.** Synthetic conditions for large-scale preparation of tebipenem pivoxil 1.

Compound 4 reaction conditions					
batch #	core 2	side chain 3	molar ratio	yield %	m.p. ( $^\circ\text{C}$ )
1	25.7 g, 43.2 mmol	10 g, 47.5 mmol	1:1.1	95	160 dec.
2	8.0 g, 13.5 mmol	3.1 g, 14.7 mmol	1:1.1	96	160 dec.
3	139.4 g, 234.5 mmol	54.3 g, 257.7 mmol	1:1.1	96	160 dec.
Compound 5 reaction conditions					
batch #	PNB ester 4	7% Pd-C	molar ratio	yield %	m.p. ( $^\circ\text{C}$ )
1	1.4 g, 2.7 mmol	0.83 g		58	186 dec.
2	5.1 g, 9.8 mmol	3.3 g		65	186 dec.
3	70 g, 135.0 mmol	41.7 g		58	186 dec.
Compound 1 reaction conditions					
batch #	compt. 5 tetrahydrate	chloromethyl pivalate	molar ratio	yield %	m.p. ( $^\circ\text{C}$ )
1	1.9 g, 4.2 mmol	1.3 g, 8.6 mmol	1:2.05	77	134-136
2	28.6 g, 62.8 mmol	19.4 g, 128.8 mmol	1:2.05	77	134-136

### 2. $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, and IR spectra of tebipenem pivoxil 1:





**Table S2.** Selected bond lengths (Å) and bond angles (°) for tebipenem pivoxil **1**.

<b>Bond</b>	<b>Dist.</b>	<b>Bond</b>	<b>Dist.</b>	<b>Bond</b>	<b>Dist.</b>
S(1)-C(5)	1.734(4)	N(1)-C(6)	1.411(5)	C(4)-C(9)	1.525(6)
S(1)-C(11)	1.799(4)	N(1)-C(1)	1.413(5)	C(4)-C(5)	1.531(5)
S(2)-C(14)	1.779(4)	N(1)-C(3)	1.478(4)	C(5)-C(6)	1.343(5)
S(2)-C(16)	1.812(7)	N(2)-C(14)	1.315(6)	C(6)-C(10)	1.471(5)
O(1)-C(1)	1.194(5)	N(2)-C(12)	1.475(6)	C(7)-C(8)	1.513(5)
O(2)-C(7)	1.409(5)	N(2)-C(13)	1.477(6)	C(11)-C(13)	1.544(6)
O(3)-C(10)	1.197(5)	N(3)-C(14)	1.259(6)	C(11)-C(12)	1.548(5)
O(4)-C(10)	1.353(5)	N(3)-C(15)	1.484(6)	C(15)-C(16)	1.475(10)
O(4)-C(17)	1.432(5)	C(1)-C(2)	1.530(5)	C(18)-C(19)	1.522(7)
O(5)-C(18)	1.332(6)	C(2)-C(7)	1.499(6)	C(19)-C(21)	1.480(9)
O(5)-C(17)	1.371(6)	C(2)-C(3)	1.552(4)	C(19)-C(22)	1.498(12)
O(6)-C(18)	1.192(6)	C(3)-C(4)	1.553(5)	C(19)-C(20)	1.498(13)
<b>Angle</b>	<b>(°)</b>	<b>Angle</b>	<b>(°)</b>	<b>Angle</b>	<b>(°)</b>
C(5)-S(1)-C(11)	102.8(2)	N(1)-C(3)-C(2)	88.5(2)	O(4)-C(10)-C(6)	111.8(3)
C(14)-S(2)-C(16)	88.8(2)	N(1)-C(3)-C(4)	104.6(3)	C(13)-C(11)-C(12)	87.3(3)
C(10)-O(4)-C(17)	116.1(4)	C(2)-C(3)-C(4)	123.6(3)	C(13)-C(11)-S(1)	114.7(2)
C(18)-O(5)-C(17)	119.9(4)	C(9)-C(4)-C(5)	110.1(4)	C(12)-C(11)-S(1)	107.7(3)
C(6)-N(1)-C(1)	132.4(3)	C(9)-C(4)-C(3)	115.9(3)	N(2)-C(12)-C(11)	88.1(3)
C(6)-N(1)-C(3)	108.6(3)	C(5)-C(4)-C(3)	100.8(3)	N(2)-C(13)-C(11)	88.1(3)
C(1)-N(1)-C(3)	93.3(3)	C(6)-C(5)-C(4)	110.3(3)	N(3)-C(14)-N(2)	125.0(4)
C(14)-N(2)-C(12)	128.6(4)	C(6)-C(5)-S(1)	125.8(3)	N(3)-C(14)-S(2)	117.4(3)
C(14)-N(2)-C(13)	130.6(4)	C(4)-C(5)-S(1)	123.7(2)	N(2)-C(14)-S(2)	117.3(3)
C(12)-N(2)-C(13)	92.6(3)	C(5)-C(6)-N(1)	111.2(3)	C(16)-C(15)-N(3)	111.2(5)
C(14)-N(3)-C(15)	111.2(4)	C(5)-C(6)-C(10)	124.8(4)	C(15)-C(16)-S(2)	105.2(4)
O(1)-C(1)-N(1)	131.7(4)	N(1)-C(6)-C(10)	124.0(3)	O(5)-C(17)-O(4)	107.8(4)
O(1)-C(1)-C(2)	136.5(4)	O(2)-C(7)-C(2)	108.4(3)	O(6)-C(18)-O(5)	120.9(5)
N(1)-C(1)-C(2)	91.8(3)	O(2)-C(7)-C(8)	111.1(3)	O(6)-C(18)-C(19)	126.6(5)
C(7)-C(2)-C(1)	118.7(3)	C(2)-C(7)-C(8)	111.2(3)	O(5)-C(18)-C(19)	112.5(4)
C(7)-C(2)-C(3)	117.8(3)	O(3)-C(10)-O(4)	123.9(3)		
C(1)-C(2)-C(3)	86.0(3)	O(3)-C(10)-C(6)	124.2(3)		