

Synthesis of Antitumor Azolato-Bridged Dinuclear Platinum(II) Complexes with In Vivo Antitumor Efficacy and Unique In Vitro Cytotoxicity Profiles

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Table S1. Crystallographic data for [*cis*-Pt(NH₃)₂]₂(μ-OH)(μ-5-methyl tetrazolato-*N2,N3*)](NO₃)₂ (**1**).

| | |
|--|---|
| Empirical formula | C ₂ H ₁₆ N ₁₀ O ₇ Pt ₂ |
| Formula weight | 682.43 |
| Crystal system | monoclinic |
| Space group | P2 ₁ /a |
| <i>a</i> [Å] | 6.760(10) |
| <i>b</i> [Å] | 12.76(3) |
| <i>c</i> [Å] | 18.06(3) |
| β [°] | 92.31(4) |
| <i>V</i> [Å ³] | 1557(5) |
| <i>Z</i> | 4 |
| ρ_{calc} [g/cm ³] | 2.912 |
| μ [mm ⁻¹] | 18.003 |
| Crystal color | colorless |
| Crystal size [mm ³] | 0.2 × 0.2 × 0.1 |
| No. of reflections measured | 11505 |
| No. of independent reflections | 3483 |
| Completeness to $\theta = 31.31^\circ$ | 88.4% |
| Refinement method | Full-matrix least-squares on F^2 |
| No. of parameters / restraints | 195 / 0 |
| Goodness-of-fit on F^2 | 1.034 |
| <i>R</i> 1 (all reflections [$I > 2\sigma(I)$]) | 0.0466 |
| <i>R</i> 1 (observed reflections [$I > 2\sigma(I)$]) | 0.0418 |
| <i>wR</i> 2 (all reflections) | 0.1247 |

| | |
|---|----------------|
| $wR2$ (observed reflections) | 0.1215 |
| Residual density [$e\text{\AA}^{-3}$] | -1.864 / 3.224 |

Table S2. Bond lengths [\AA] and angles [$^\circ$] for **1**.

| | |
|---------|-----------|
| Pt1—N2 | 1.975(9) |
| Pt1—N6 | 2.025(9) |
| Pt1—N7 | 2.039(9) |
| Pt1—O1 | 2.034(8) |
| Pt2—N3 | 1.978(10) |
| Pt2—N9 | 2.029(10) |
| Pt2—N8 | 2.039(12) |
| Pt2—O1 | 2.028(7) |
| N1—N2 | 1.326(11) |
| N1—C5 | 1.349(16) |
| N2—N3 | 1.337(17) |
| N3—N4 | 1.343(12) |
| N4—C5 | 1.337(17) |
| C5—C51 | 1.502(16) |
| N11—O12 | 1.189(16) |
| N11—O13 | 1.178(18) |
| N11—O14 | 1.29(2) |
| N21—O22 | 1.245(14) |
| N21—O23 | 1.29(3) |
| N21—O24 | 1.214(19) |

| | |
|-------------|-----------|
| N2—Pt1—N6 | 90.4(3) |
| N2—Pt1—O1 | 87.8(3) |
| N2—Pt1—N7 | 179.8(3) |
| N6—Pt1—N7 | 89.5(3) |
| N7—Pt1—O1 | 92.3(3) |
| N6—Pt1—O1 | 178.3(3) |
| N3—Pt2—N9 | 90.8(4) |
| N3—Pt2—O1 | 88.4(3) |
| N3—Pt2—N8 | 179.2(4) |
| N8—Pt2—N9 | 89.6(5) |
| N8—Pt2—O1 | 91.1(4) |
| N9—Pt2—O1 | 179.2(4) |
| C5—N1—N2 | 103.6(9) |
| N1—N2—N3 | 110.4(8) |
| N1—N2—Pt1 | 126.4(6) |
| N3—N2—Pt1 | 123.2(6) |
| N2—N3—N4 | 109.3(8) |
| N2—N3—Pt2 | 121.6(6) |
| N4—N3—Pt2 | 129.0(7) |
| C5—N4—N3 | 103.6(9) |
| N1—C5—N4 | 112.8(10) |
| N1—C5—C51 | 124.2(14) |
| N4—C5—C51 | 123.0(13) |
| Pt2—O1—Pt1 | 116.2(3) |
| O12—N11—O13 | 131(2) |
| O12—N11—O14 | 115.1(17) |
| O13—N11—O14 | 114.3(17) |

O22—N21—O23 114.7(13)

O22—N21—O24 126.9(17)

O23—N21—O24 117.9(15)
