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SUPPLEMENTARY MATERIAL TO

Novel methylene bridged ethylenediamine-type ligands: synthesis and spectral characterization

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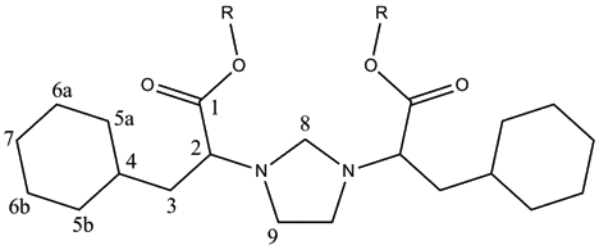

R= *i*Bu *i*Pe
C1 C2

Structures of **C1** and **C2** with atomic numbering.

ANALYTIC AND SPECTRAL DATA FOR **C1** AND **C2**

*Compound **C1***. Yield: 83 %; Anal. Calcd. for $C_{29}H_{52}N_2O_4$: C, 70.69, H, 10.64, N, 5.69 %. Found: C, 70.38; H, 10.36; N, 5.76 %; IR (ATR, cm^{-1}): 2928, 2852, 1734, 1468, 1451, 1375, 1252, 1165, 994; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / / ppm): 0.82–0.90 (4H, *m*, H5a′, H5b′), 0.92 (12H, *d*, *J* = 7.0 Hz, $(CH_3)_2CH$), 1.07–1.31 (8H, *m*, H4, H7′, H6b), 1.47–1.52 (2H, *m*, CH_2′Cy), 1.60–1.66 (10H, *m*, H6a, H5a, H7, CH_2Cy), 1.76 (2H, *d*, *J* = 12.5 Hz, H5b), 1.92 (2H, *m*, $(CH_3)_2CHCH_2O$), 2.82–2.88 (2H, *m*, NCH_2CH_2N), 2.95–3.01 (2H, *m*, NCH_2CH_2N), 3.36–3.39 (2H, *m*, OCCHN), 3.63 (2H, *s*, NCH_2N), 3.86 (4H, *d*, *J* = 6.5 Hz, CH_2OOC); ^{13}C-NMR (125 MHz, $CDCl_3$, δ / ppm): 19.29 ($(CH_3)_2CH$), 26.25 (C6a), 26.28 (C6b), 26.59 (C7), 27.80 ($(CH_3)_2CH$), 33.20 (C5b), 33.74 (C5a), 34.50 (C4), 38.89 (CH_2Cy), 48.23 (NCH_2CH_2N), 62.05 (OCCHN), 69.55 (NCH_2N), 70.59 (CH_2OOC), 173.31 (C1). ESI-MS (*m*/*z*, (relative abundance, %)): 481.58 ($M–CH_2+3H^+$, 100), 493.40 (M^+, 37.16).

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Compound ***C2***. Yield: 71 %; Anal. Calcd. for $C_{31}H_{56}N_2O_4$: C, 71.49, H, 10.84, N, 5.38 %. Found: C, 71.10; H, 10.44; N, 5.49 %; IR (ATR, cm^{-1}): 2924, 2851, 1732, 1683, 1449, 1367, 1306, 1252, 1164, 971; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm) 0.82–0.88 (4H, *m*, H5a′, H5b′), 0.90 (12H, *d*, *J* = 6.5 Hz, (C**H**$_3$)$_2$CH), 1.06–1.31 (8H, *m*, H4, H7′, H6b), 1.46–1.53 (2H, *m*, CH_2′Cy), 1.59––1.70 (10H, *m*, H6a, H5a, H7, CH_2Cy), 1.75 (2H, *d*, *J* = 13.0 Hz, H5b), 2.80––2.86 (2H, *m*, NCH_2C**H**$_2$N), 2.94–3.00 (2H, *m*, NC**H**$_2$CH_2N), 3.33–3.35 (2H, *m*, OCCHN), 3.61 (2H, *s*, NCH_2N), 4.11 (4H, *m*, CH_2C**H**$_2$OOC); ^{13}C-NMR (50 MHz, $CDCl_3$, δ / ppm): 11.32 and 16.61 ((**C**H$_3$)$_2$CH), 22.56 ((CH$_3$)$_2$**C**H), 25.16 (C6a), 26.27 (C6b), 26.60 (C7), 33.19 (C5b), 33.77 (C5a), 34.52 (C4), 37.50 ((CH$_3$)$_2$CH**C**H$_2$), 38.87 (**C**H$_2$Cy), 48.30 (N**C**H$_2$**C**H$_2$N), 62.16 (OC**C**HN), 63.04 (**C**H$_2$OOC), 69.60 (NCH$_2$N), 173.47 (C1); ESI-MS (*m*/*z*, (relative abundance, %)): 509.43 (M–CH$_2$+3H$^+$, 49), 521.43 (M$^+$, 100).

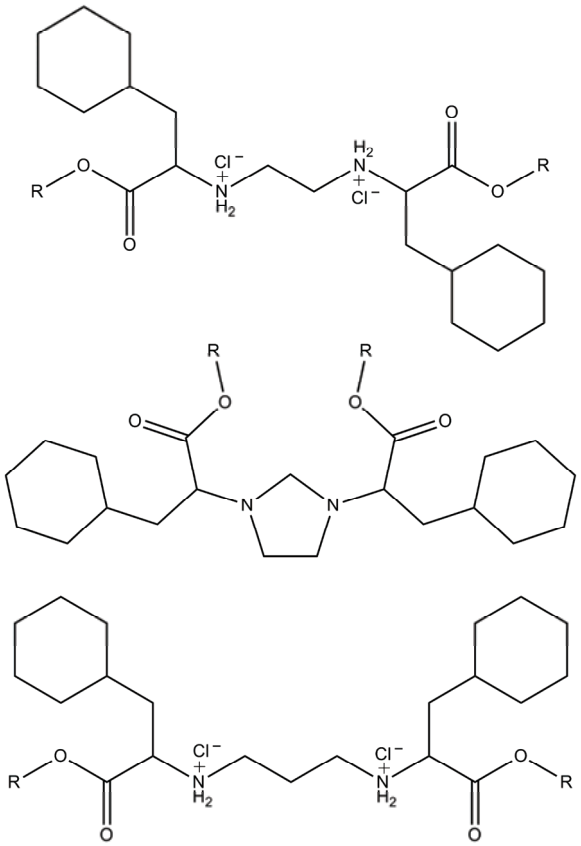

Fig. S-1. Recently synthesized compounds with confirmed antitumor activity.

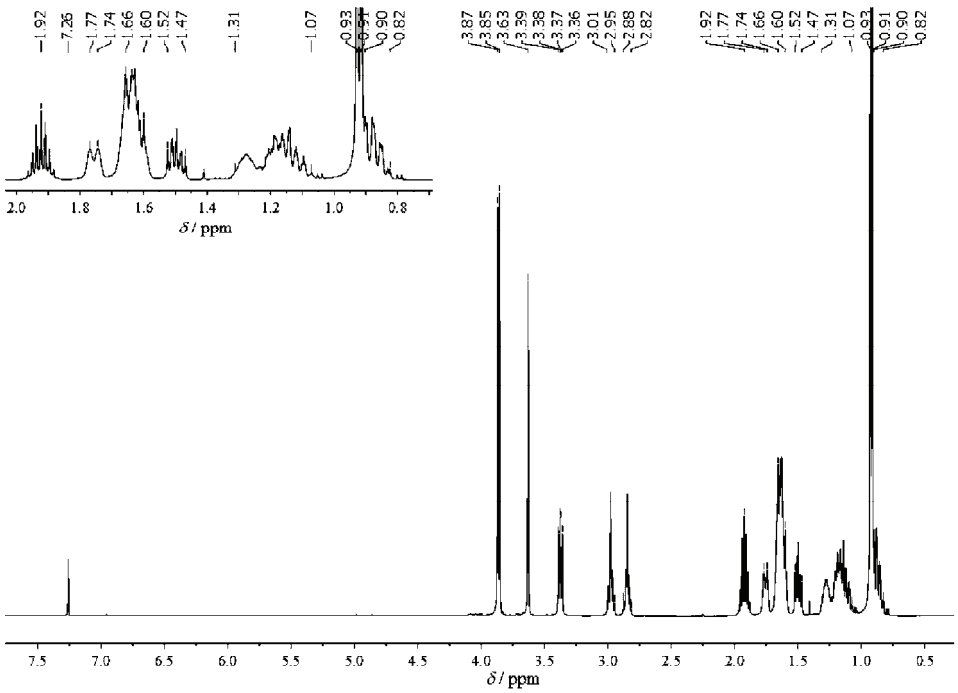

Fig. S-2. ^{1}H-NMR spectrum of **C1** recorded in $CDCl_3$

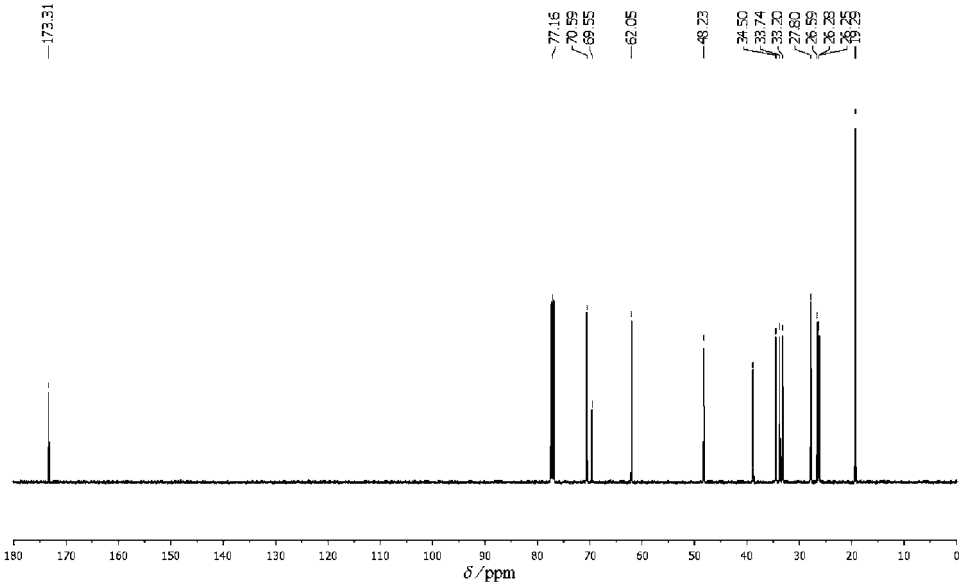

Fig. S-3. ^{13}C-NMR spectrum of **C1** recorded in $CDCl_3$.

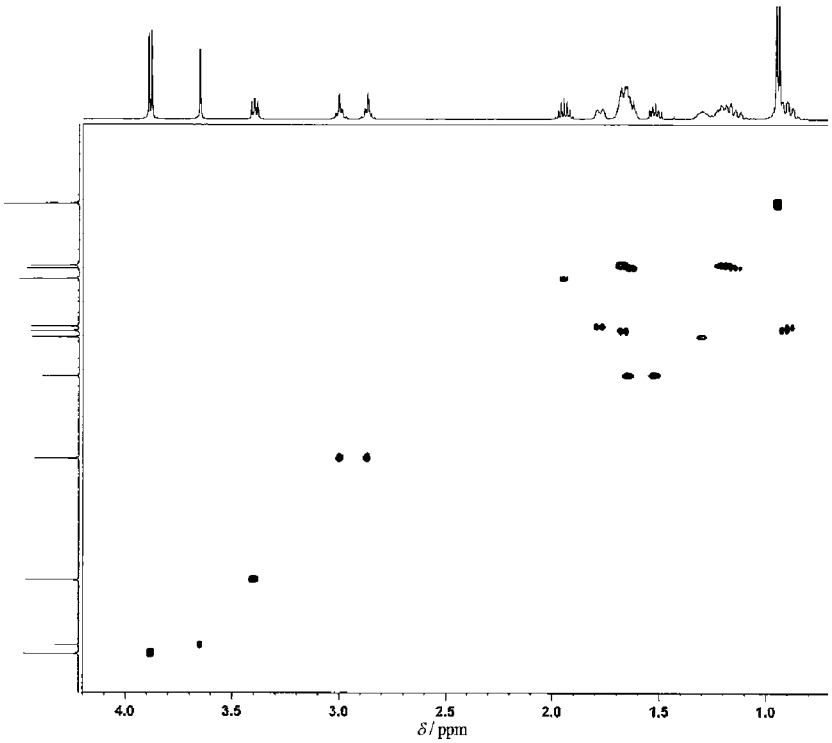

Fig. S-4. HSQC NMR spectrum of **C1** recorded in $CDCl_3$.

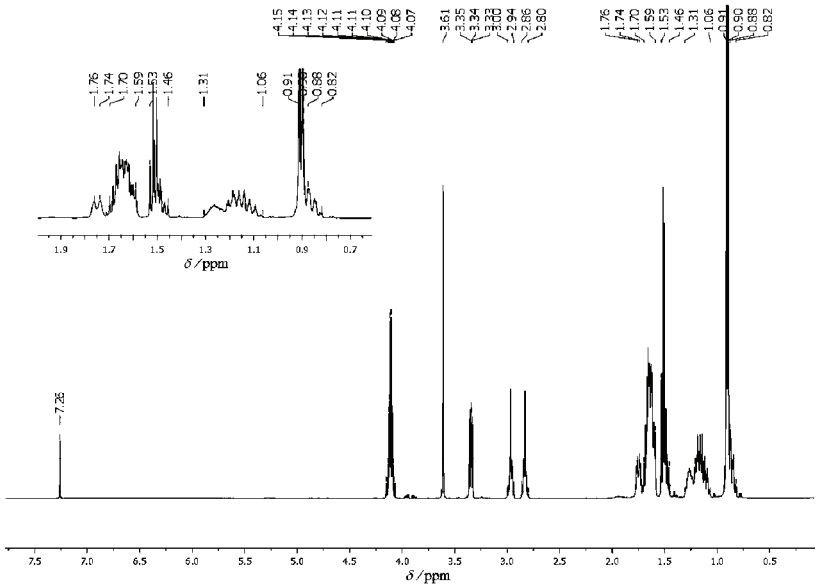

Fig. S-5. ^{1}H-NMR spectrum of **C2** recorded in $CDCl_3$.

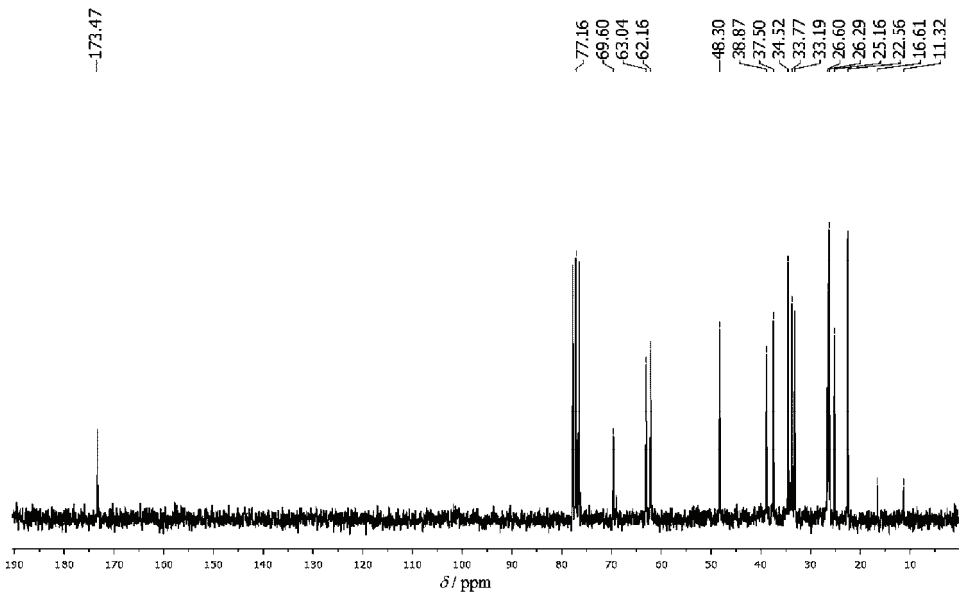

Fig. S-6. ^{13}C-NMR spectrum of **C2** recorded in $CDCl_3$.

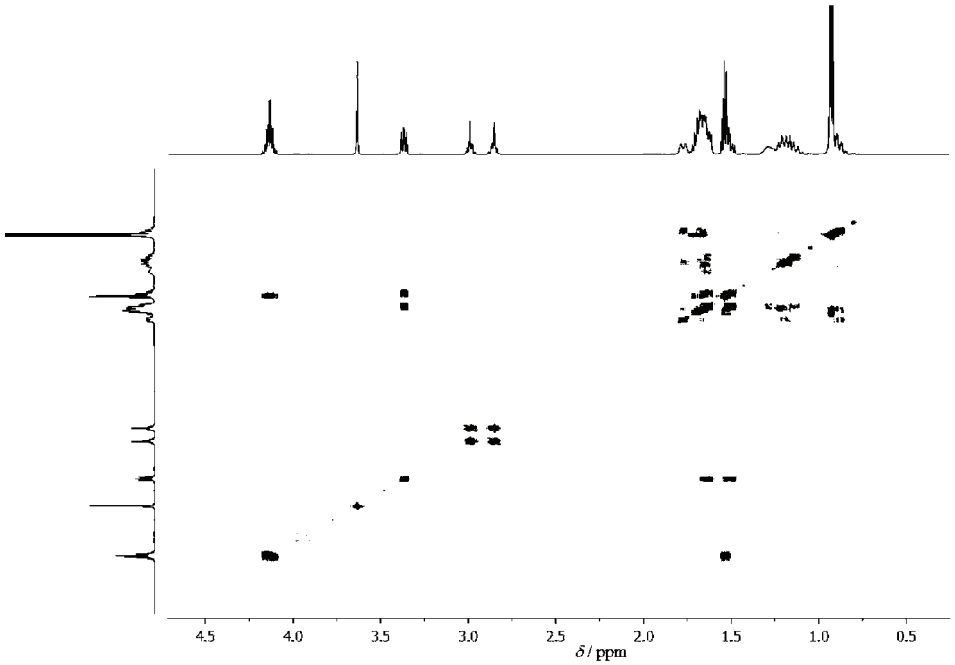

Fig. S-7. COSY NMR spectrum of **C2** recorded in $CDCl_3$.