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New anthrahydrazone derivatives and their cisplatin-like complexes: Synthesis, antitumor activity and structure-activity relationship

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Table S1. Selected bonds lengths and angles for the platinum(II) complexes **1** and **2**

Selected bond (Å)			
Pt complex **1**		Pt complex **2**	
Pt1–Cl1	2.279(2)	Pt1–Cl1	2.2854(12)
Pt1–Cl2	2.289(2)	Pt1–Cl2	2.2866(12)
Pt1–N1	1.975(7)	Pt1–N1	1.995(4)
Pt1–N4	2.001(6)	Pt1–N4	2.015(3)

Selected angles (°)			
Pt complex **1**		Pt complex **2**	
Cl1–Pt1–Cl2	88.80(9)	Cl1–Pt1–Cl2	89.06(5)
N1–Pt1–Cl1	95.9(2)	N1–Pt1–Cl1	95.78(11)
N1–Pt1–Cl2	175.26(19)	N1–Pt1–Cl2	175.14(11)
N1–Pt1–N4	80.2(3)	N1–Pt1–N4	80.61(14)
N3–N4–Pt1	112.4(4)	N3–N4–Pt1	112.4(2)
C3–N1–Pt1	129.6(7)	C3–N1–Pt1	129.4(3)
C12–C13–C14	122.4(8)	O1–C14-C13	123.1(5)

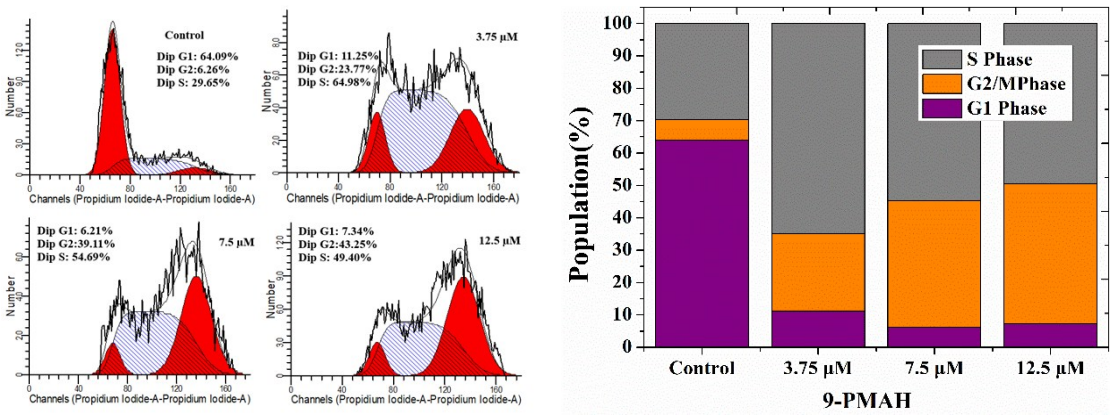


Figure S1. The percentages for the different phases of the cell cycle in T-24 cells arrested by **9-PMAH**.

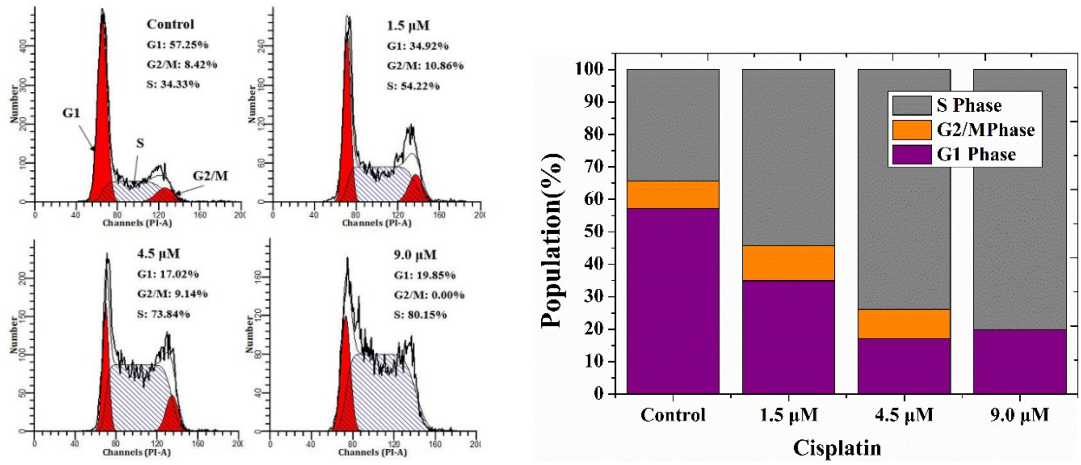


Figure S2. The percentages for the different phases of the cell cycle in T-24 cells arrested by **cisplatin**, with the same concentrations as 9-PMAH-Pt.

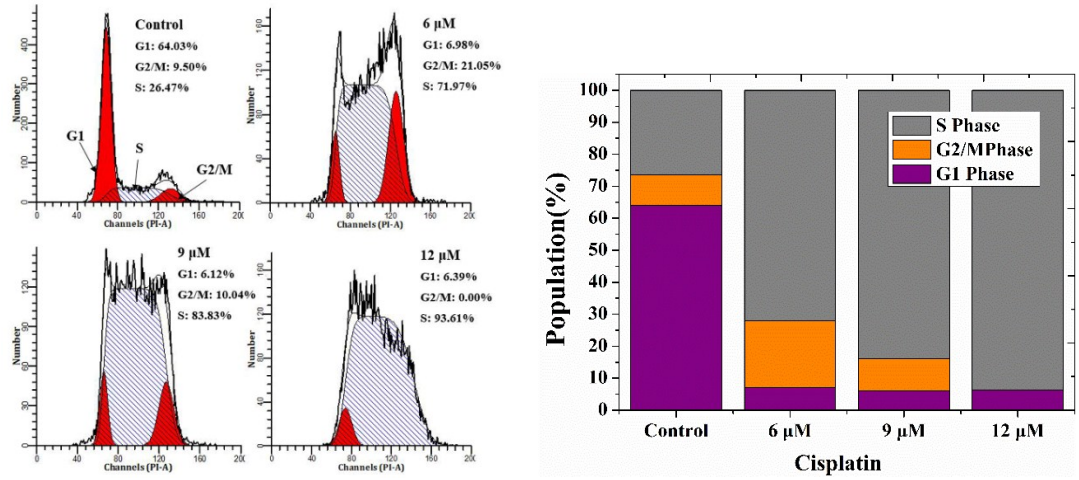


Figure S3. The percentages for the different phases of the cell cycle in MGC-803 cells arrested by **cisplatin**, with the same concentrations as 9-PMAH-Pt.

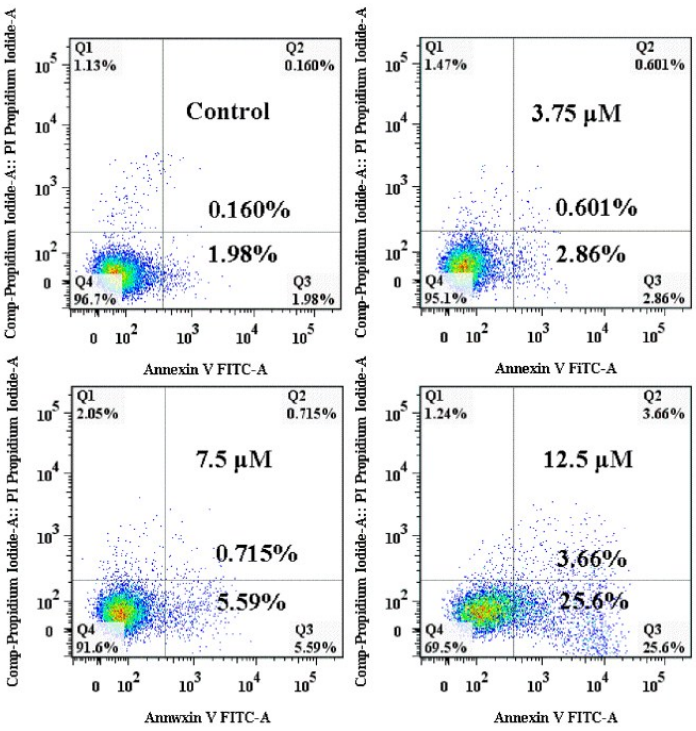


Figure S4. The cell apoptosis in T-24 cells induced by 9-PMAH in different concentrations related with IC_{50} value.

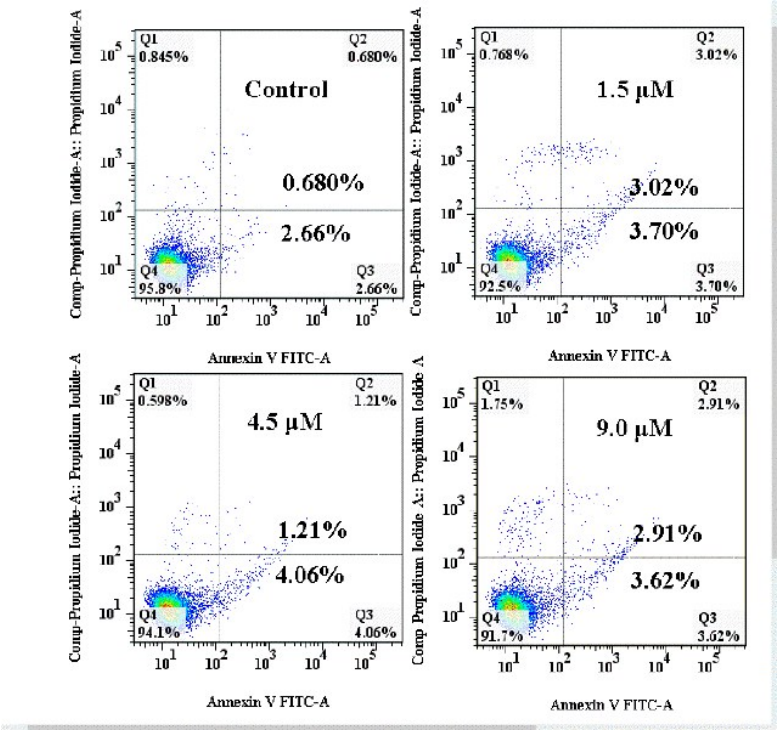


Figure S5. The cell apoptosis in T-24 cells induced by **cisplatin**, with the same concentrations as 9-PMAH-Pt

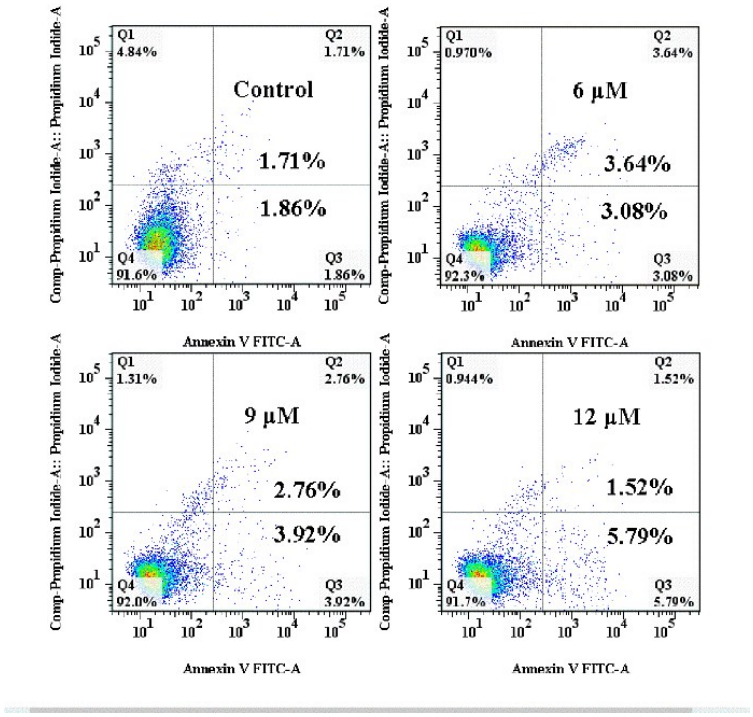


Figure S6. The cell apoptosis in MGC-803 cells induced by **cisplatin**, with the same concentrations as 9-PMAH-Pt

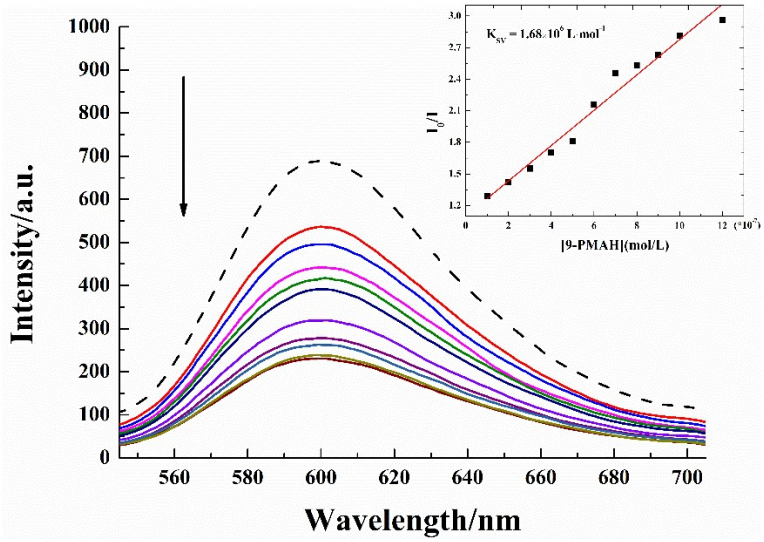


Figure S7. The fluorescence emission spectra of GR-DNA in the absence (dashed line) and the presence (solid lines) of 9-PMAH with increasing concentrations ([GR]/[DNA]/[9-PMAH] range from 1:10:0.01 to 1:10:0.09).

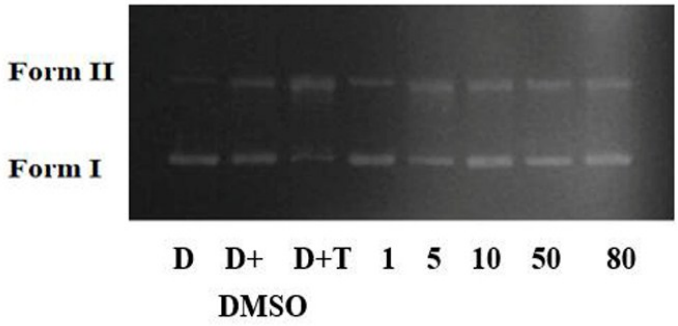
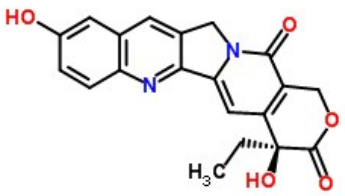
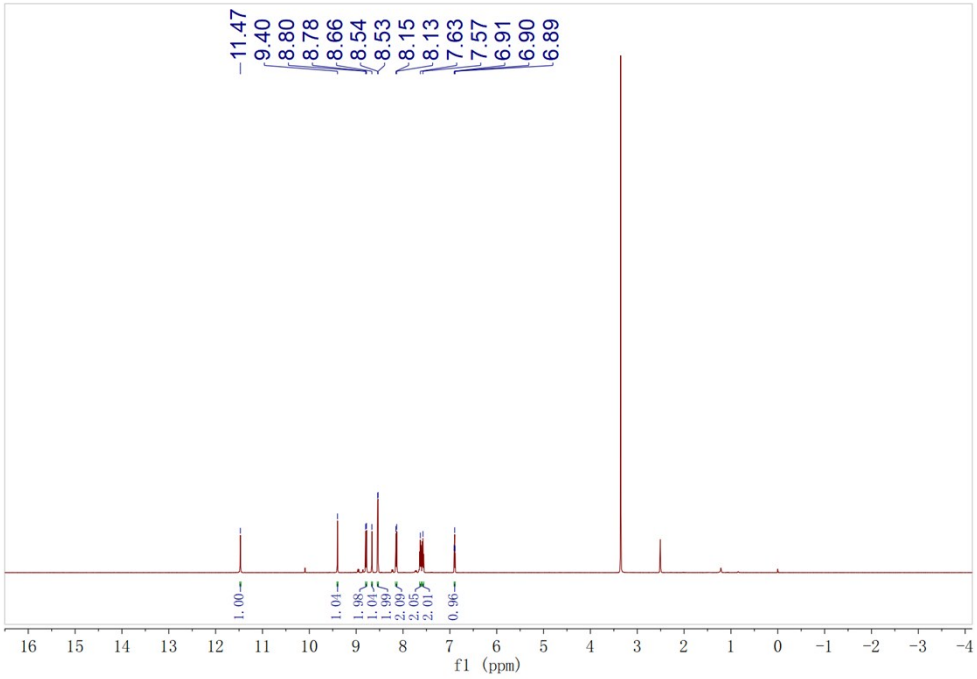


Figure S8. Inhibitory abilities of (S)-10-Hydroxycamptothecin on topoisomerase type I (Topo I)

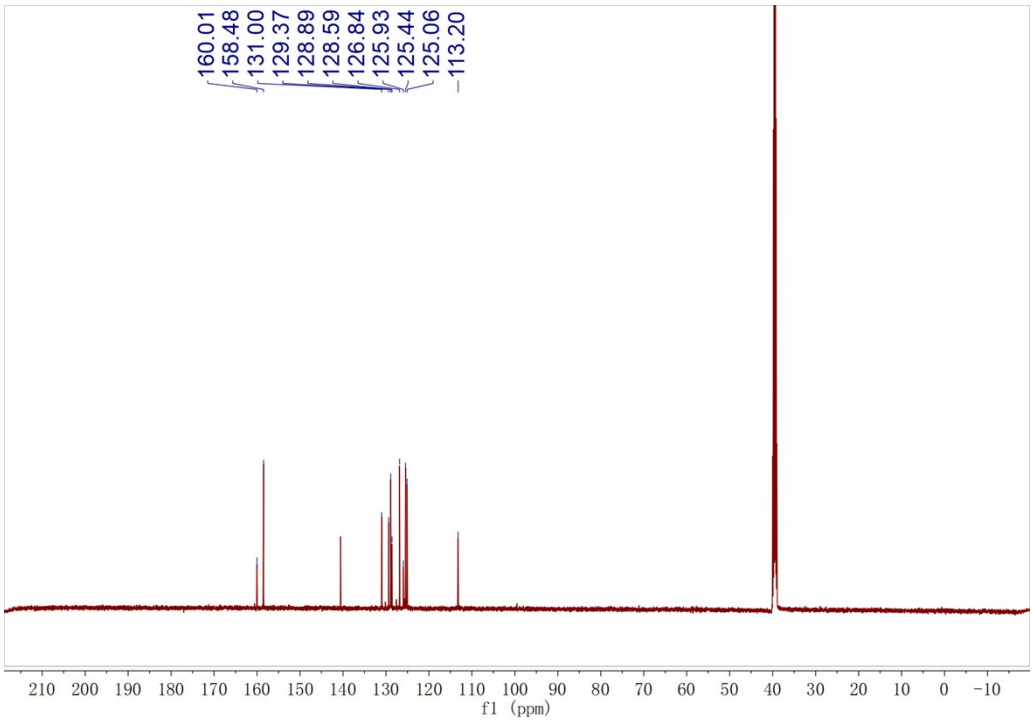


(S)-10-Hydroxycamptothecin

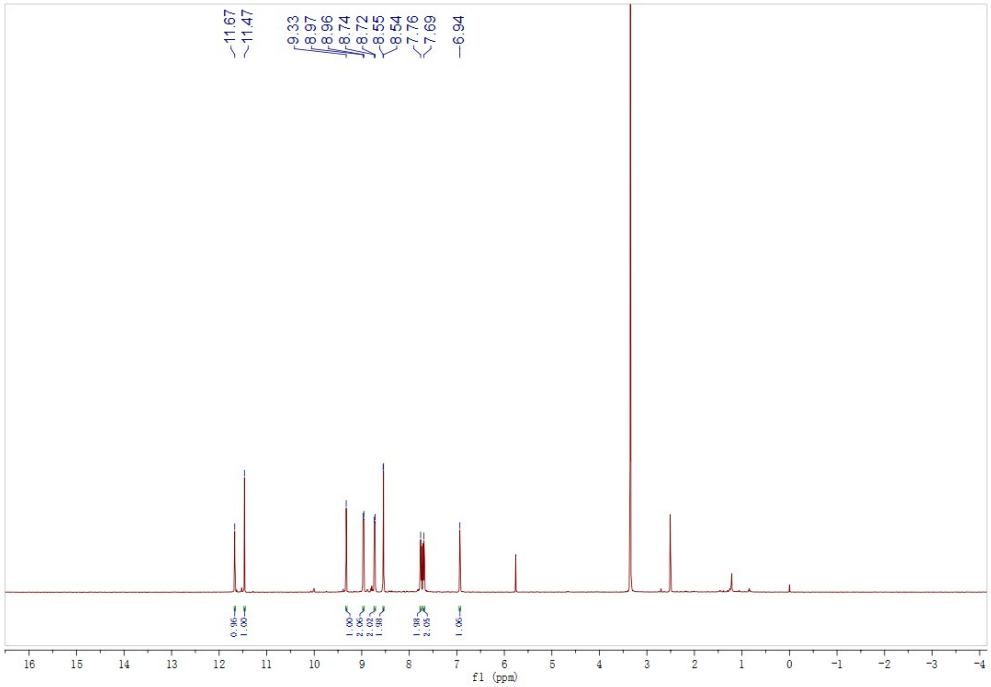
The spectral characterizations for both the ligands and both the Pt(II) complexes:



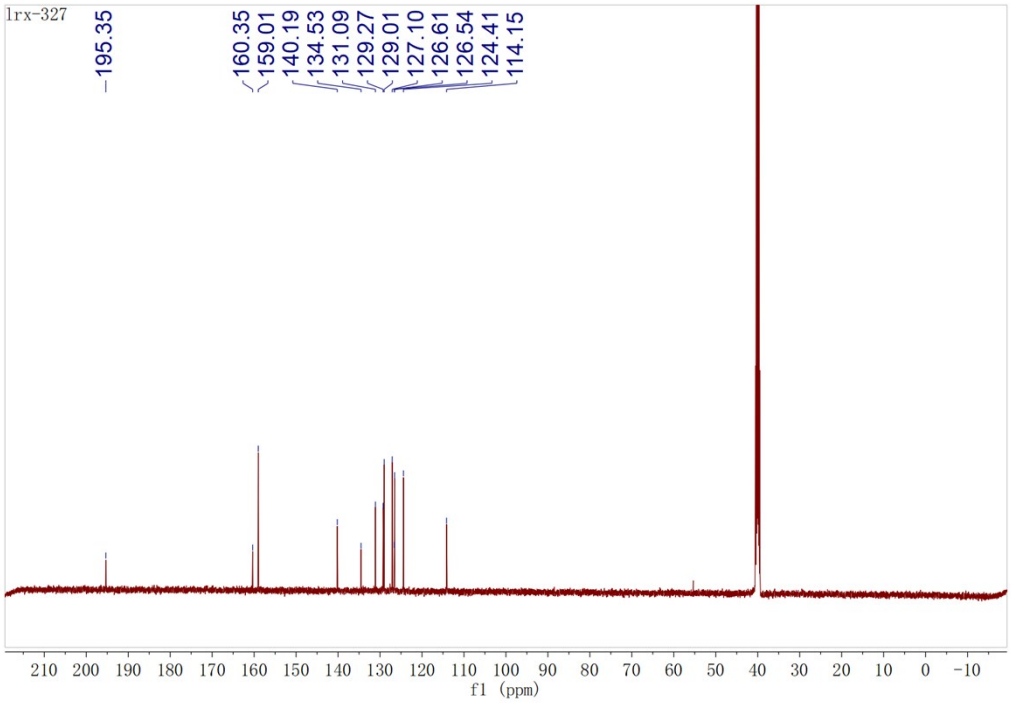
9-PMAH: ^{1}H-NMR (500 MHz, d_6-DMSO) δ 11.47 (s, 1H), 9.40 (s, 1H), 8.79 (d, J=8.9 Hz, 2H), 8.66 (s,1H), 8.54 (d, J=4.7 Hz, 2H), 8.14 (d, J=8.3 Hz, 2H), 7.63 (s, 2H), 7.57 (s, 2H), 6.90 (t, J=4.7 Hz, 1H).



9-PMAH: ^{13}C-NMR (126 MHz, d_6-DMSO) δ 160.01, 158.48, 140.55, 131.00, 129.37, 128.89, 128.59, 126.84, 125.93, 125.44, 125.06, 113.20.

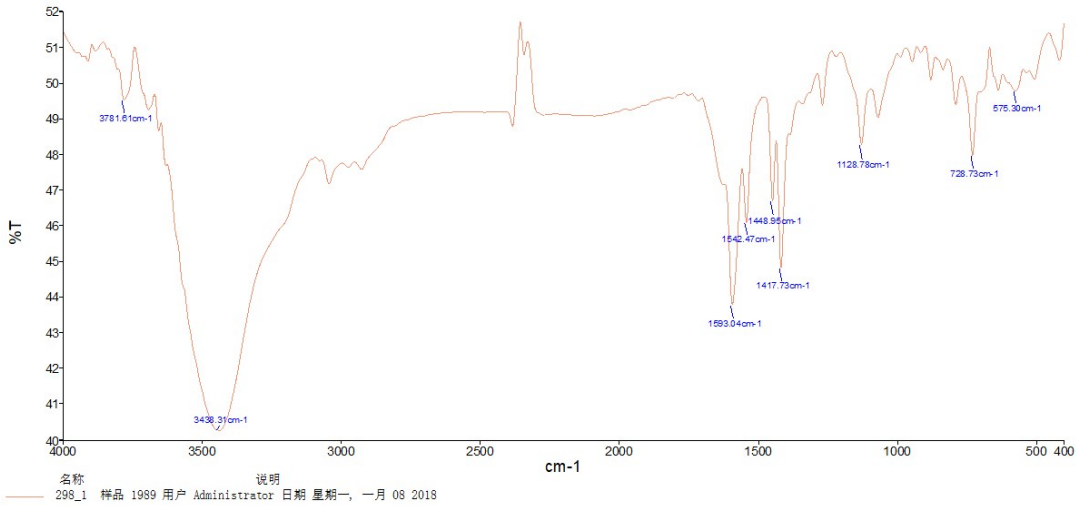


APMAH: ^{1}H NMR(500 MHz, d_6-DMSO): δ 11.67 (s, 1H), 11.47 (s, 1H), 9.33 (s, 1H), 8.96 (d, J=8.8 Hz, 2H), 8.73 (d, J=8.8 Hz, 2H), 8.55 (d, J=4.8 Hz, 2H),7.76 (s, 2H), 7.69 (s, 2H), 6.94 (t, J=4.5Hz ,1H).

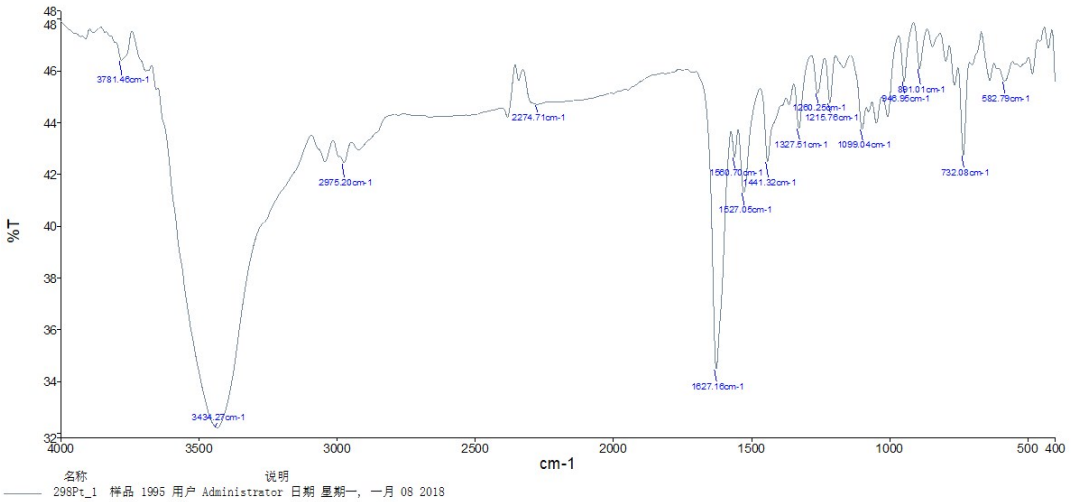


APMAH: ^{13}C NMR(126MHz, d_6-DMSO): δ 195.35, 160.35, 159.01, 140.19, 134.53,

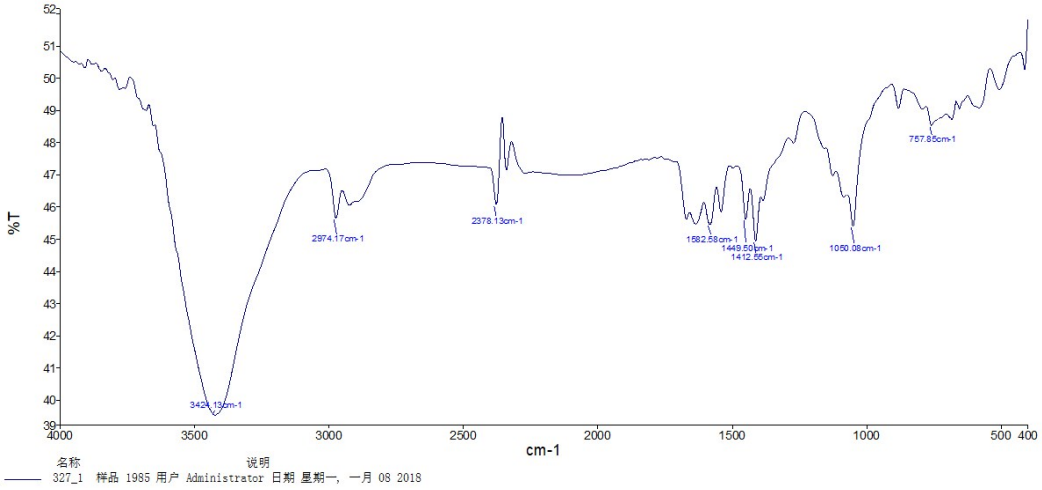
131.09, 129.27, 129.01, 127.10, 126.61, 126.54, 124.41, 114.15.



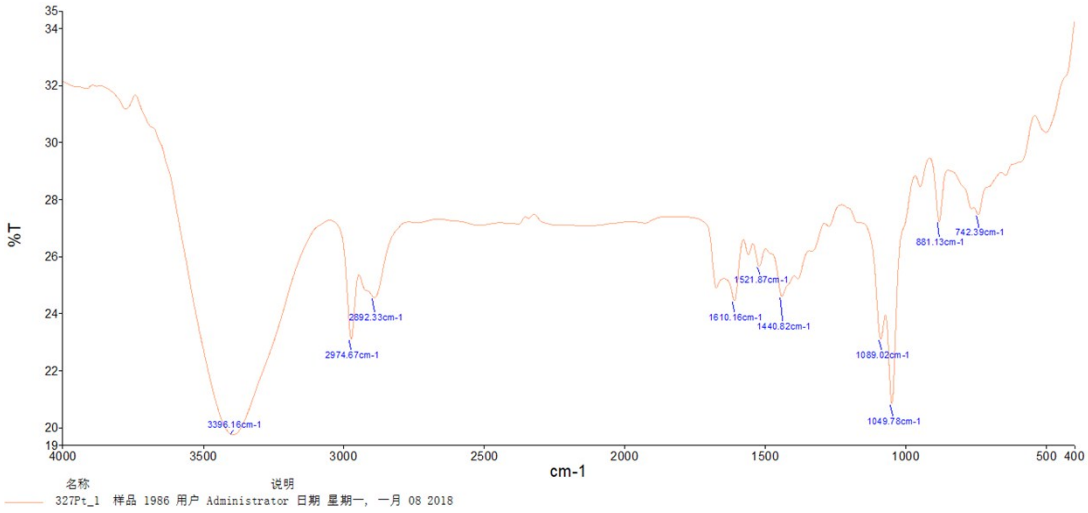
9-PMAH: IR (KBr): 3781, 3438, 1593, 1542, 1448, 1417, 1128, 728, 575 cm^{-1}



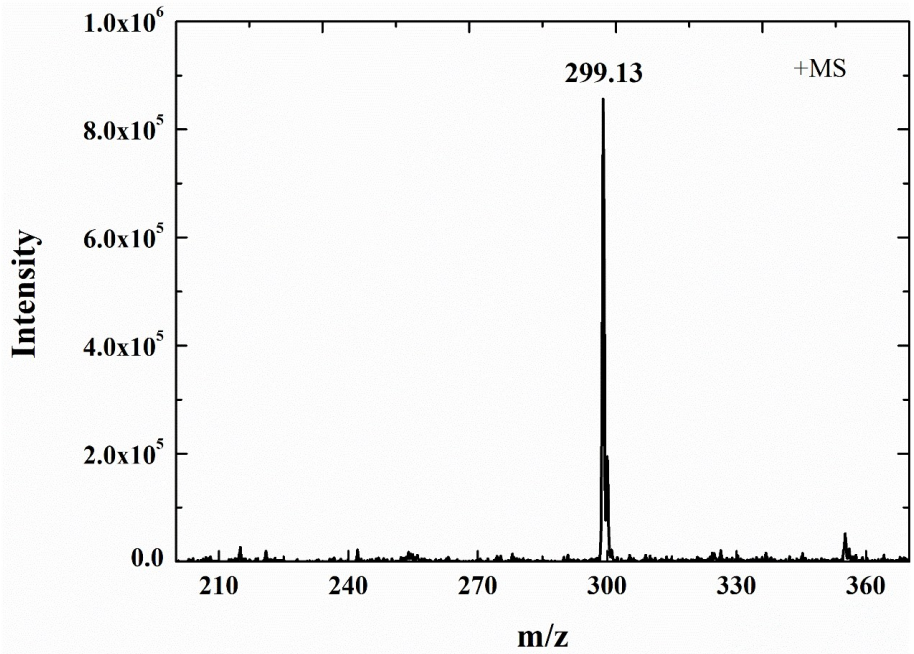
9-PMAH-Pt: IR (KBr): 3781, 3434, 2975, 2274, 1627, 1560, 1527, 1441, 1327, 1260, 1215, 1099, 946, 891, 732, 582m^{-1}.



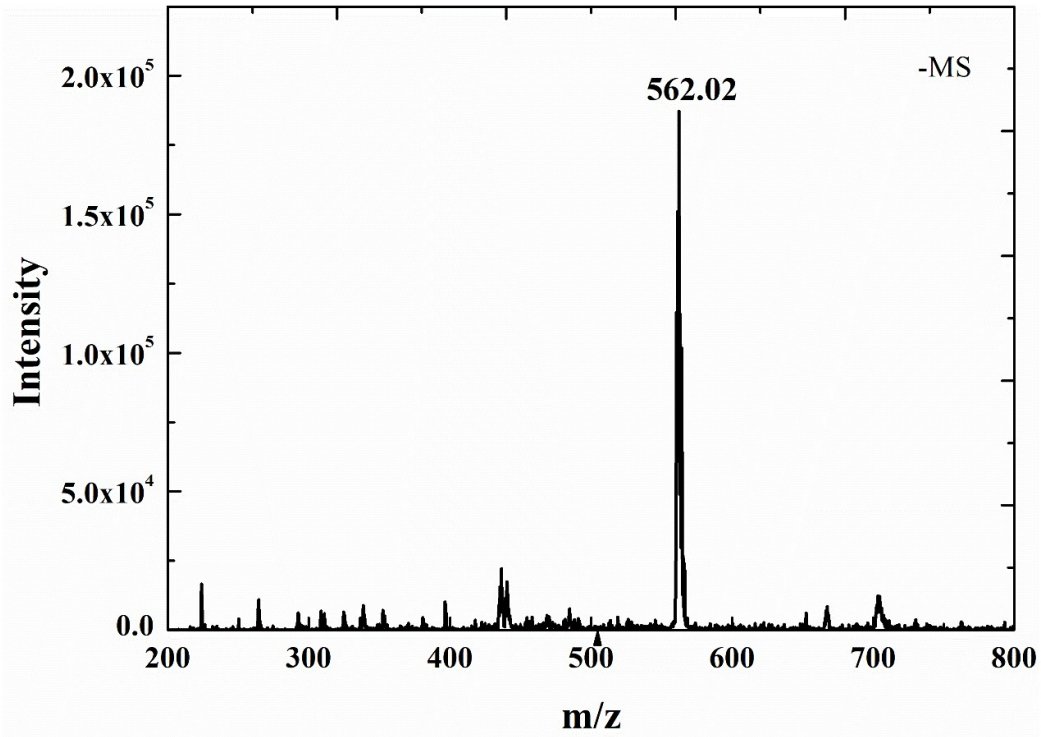
APMAH: IR (KBr): 3424, 2974, 2378, 1582, 1449, 1412, 1050, 757 cm^{-1}



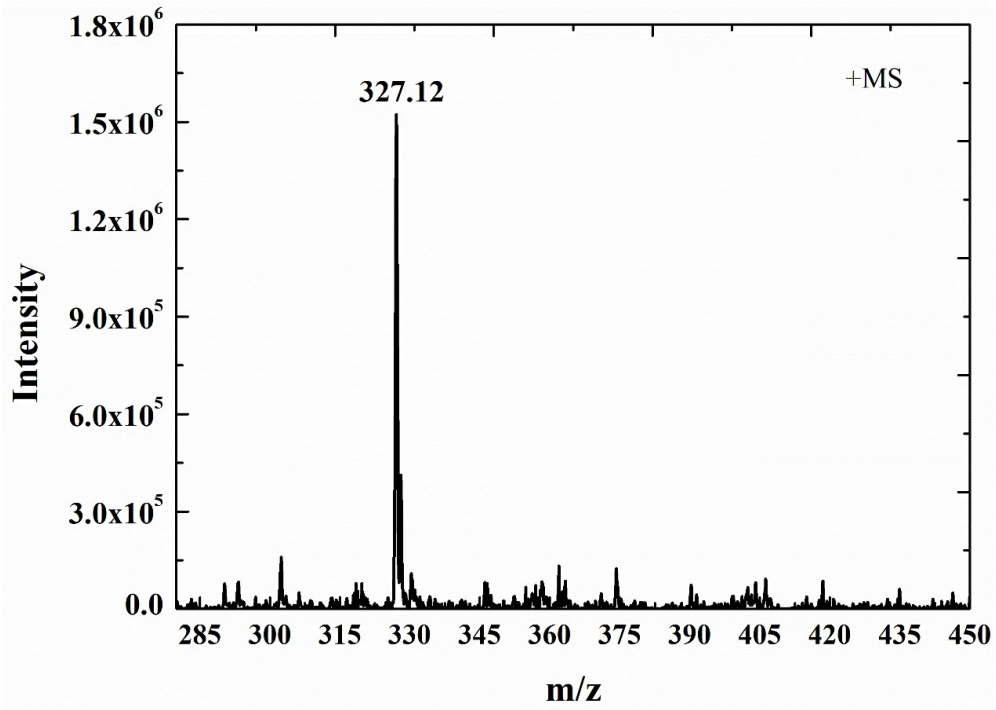
APMAH-Pt: IR (KBr): 3396, 2974, 2892, 1610, 1521, 1440, 1089, 1049, 881, 742 cm^{-1}



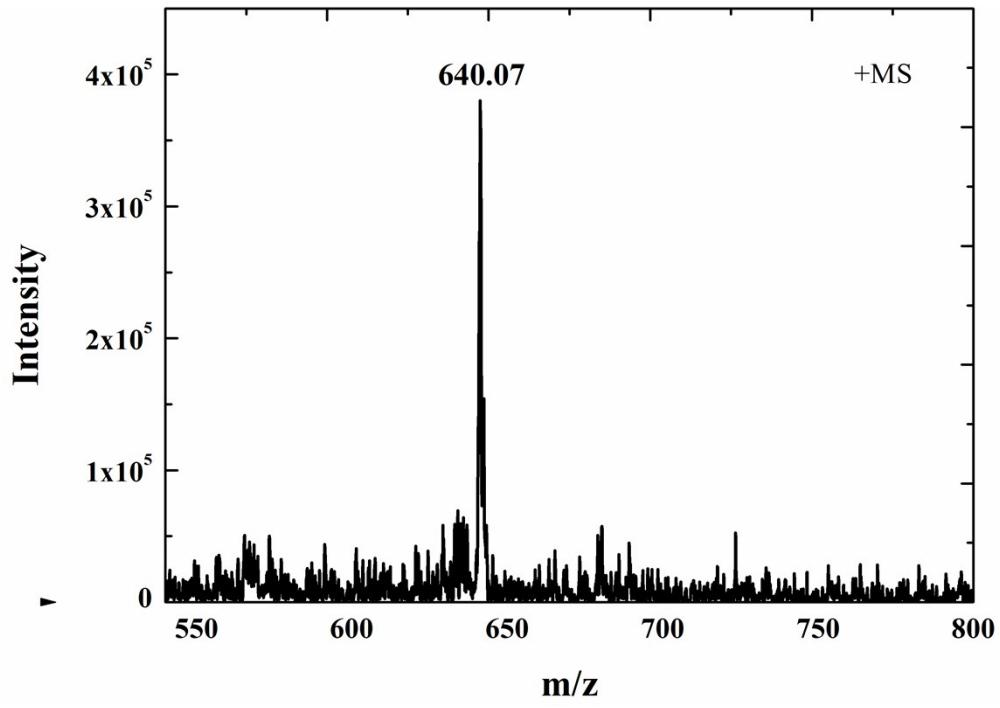
9-PMAH: m/z: 299.13 $[M+H]^+$



9-PMAH-Pt: m/z: 562.02 for $[Pt^{II}Cl_2(9\text{-PMAH})–H]^-$



APMAH: m/z: 327.12 $[M+H]^+$



APMAH-Pt: m/z: 640.07 for $[Pt^{II}Cl_2(APMAH)+EtOH+H]^+$