

New Journal of Chemistry – Supporting Information

Synthesis, G-quadruplex binding properties and cytotoxicity of naphthalimide-  
thiourea conjugates

Zhize Ou<sup>a</sup>, Moheng Xu<sup>a</sup>, Yunyan Gao<sup>\*a</sup>, Rui Hu<sup>b</sup>, Qingqing Li<sup>a</sup>, Wenjiao Cai<sup>a</sup>, Ziji  
Wang<sup>a</sup>, Yimeng Qian<sup>a</sup>, Guoqiang Yang<sup>b</sup>

(<sup>a</sup>The Key Laboratory of Space Applied Physics and Chemistry, Ministry of  
Education, Department of Applied Chemistry, School of Science, Northwestern  
Polytechnical University, Xi'an, 710072, People's Republic of China

<sup>b</sup>CAS Key laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of  
Sciences, Beijing 100190, People's Republic of China)

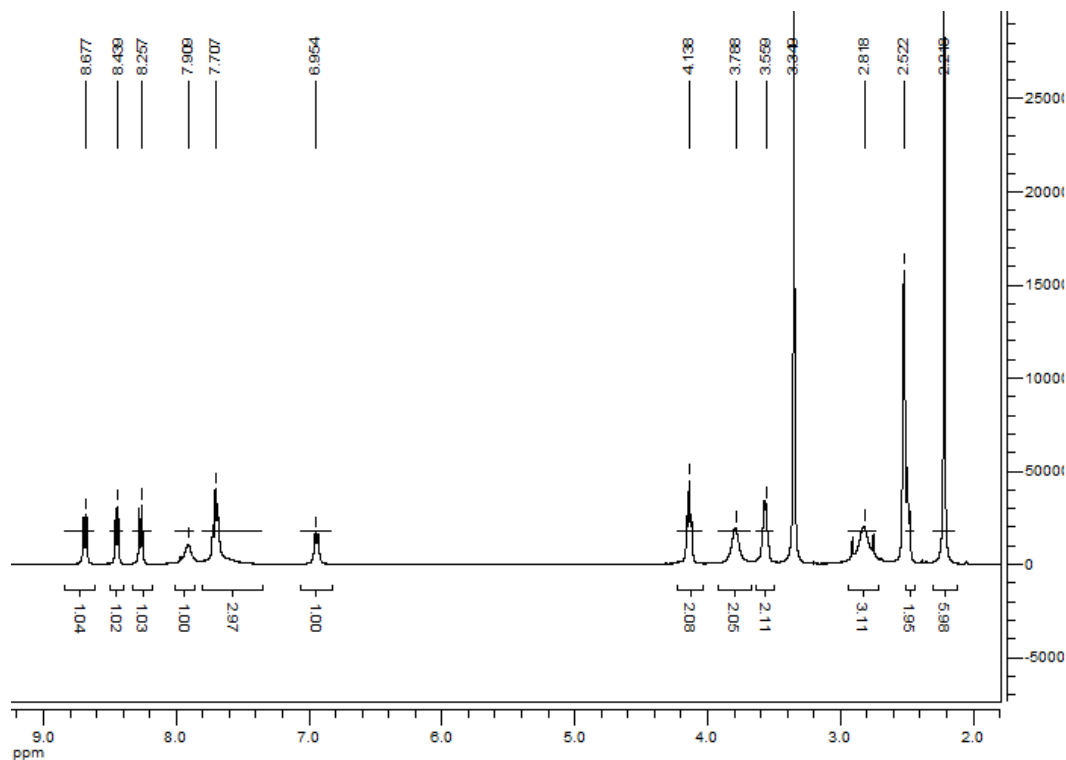
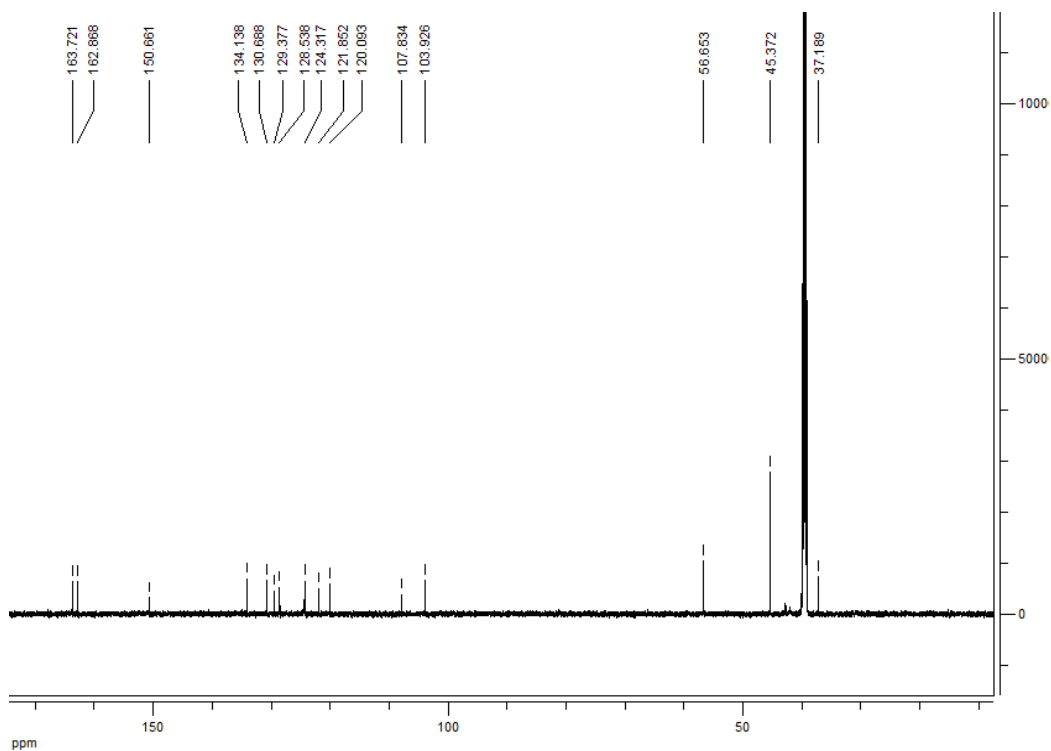


Fig. S1 <sup>1</sup>H NMR of **3a** in DMSO-d<sub>6</sub>.

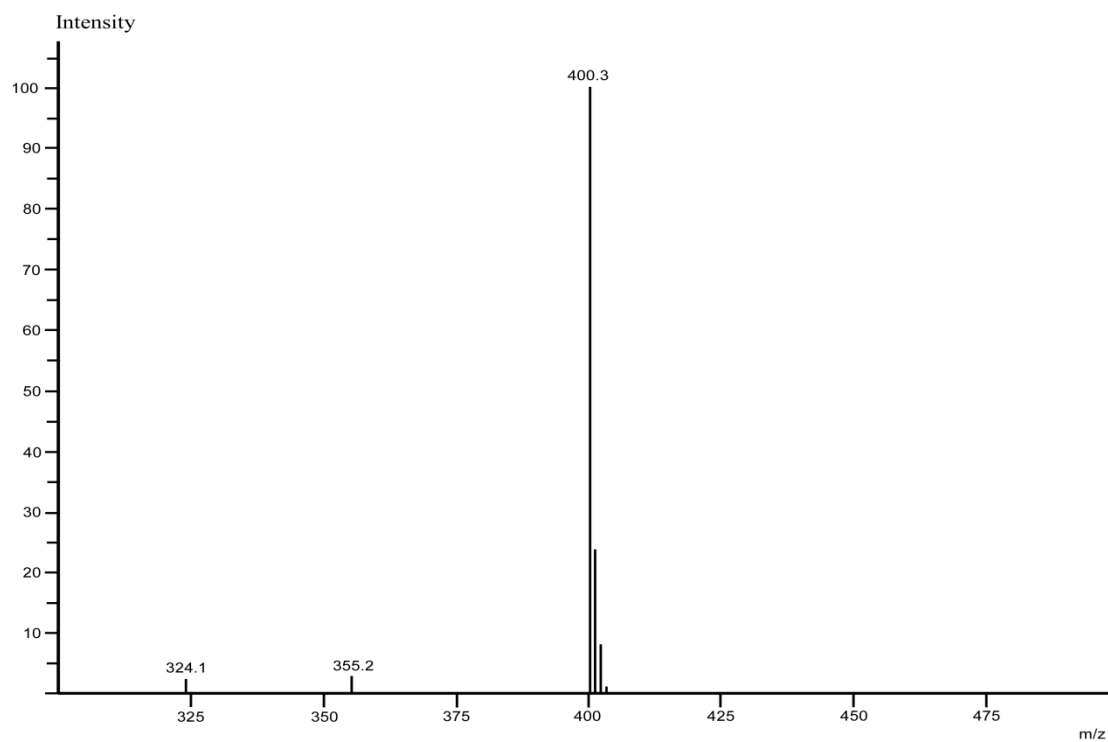


**Fig. S2**  $^{13}\text{C}$  NMR of **3a** in  $\text{DMSO-d}_6$ .

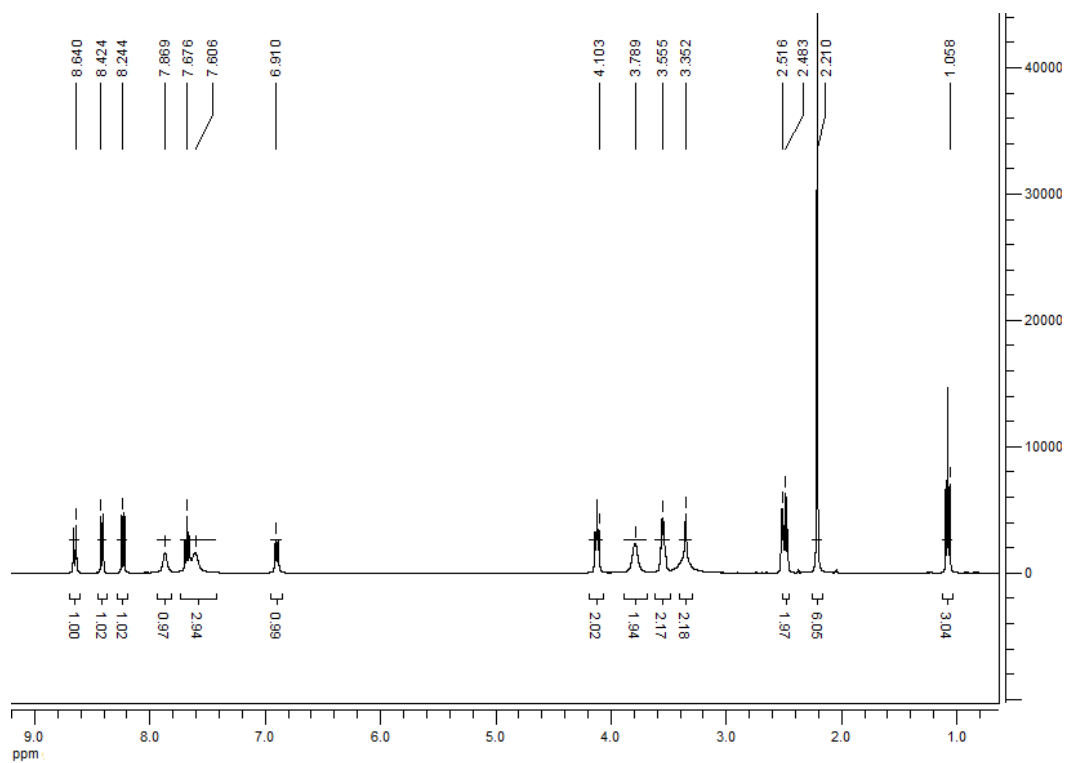
ESI-MS Spectrum, NIE-Me

#:1 Ret Time:Averaged 1.307-1.627(Scan#:50-62)

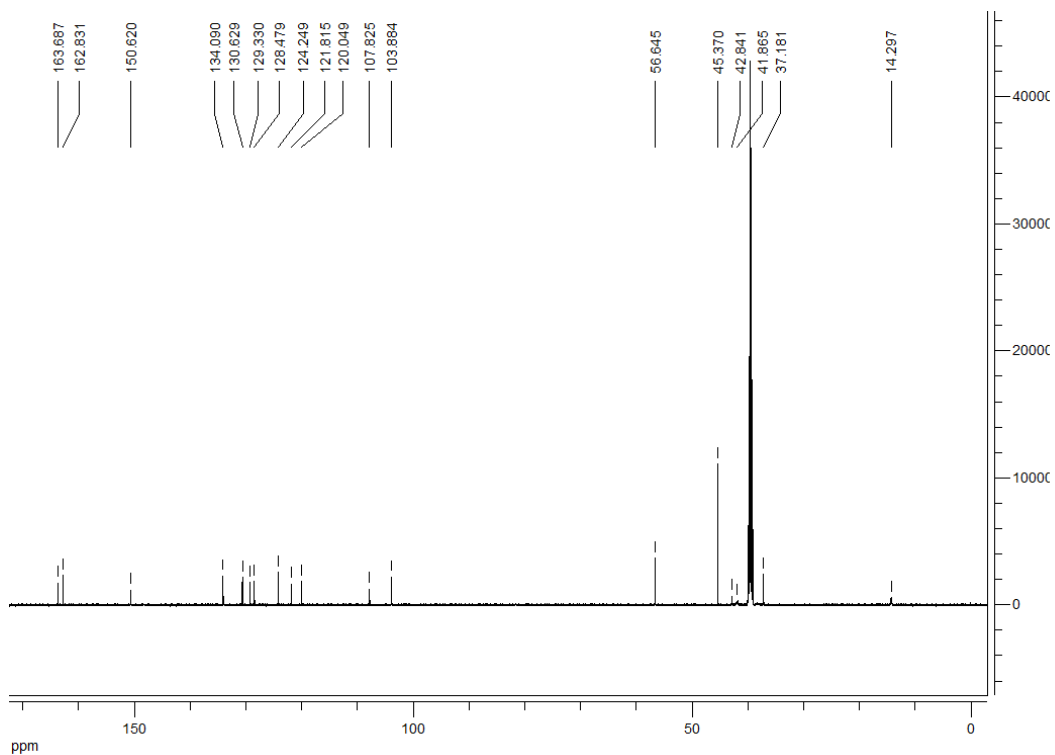
Mass Peaks:230 Base peak:400.30(3323541) Polarity:Pos Segment - Event1



**Fig. S3** ESI-MS of **3a** in  $\text{DMSO-d}_6$ .



**Fig. S4**  $^1\text{H}$  NMR of **3b** in  $\text{DMSO-d}_6$ .



**Fig. S5**  $^{13}\text{C}$  NMR of **3b** in  $\text{DMSO-d}_6$ .

ESI-MS Spectrum, NIE-Et

#:1 Ret Time:Averaged 1.307-1.653(Scan#:50-63)

Mass Peaks:206 Base peak:414.25(2901681) Polarity:Pos Segment - Event1

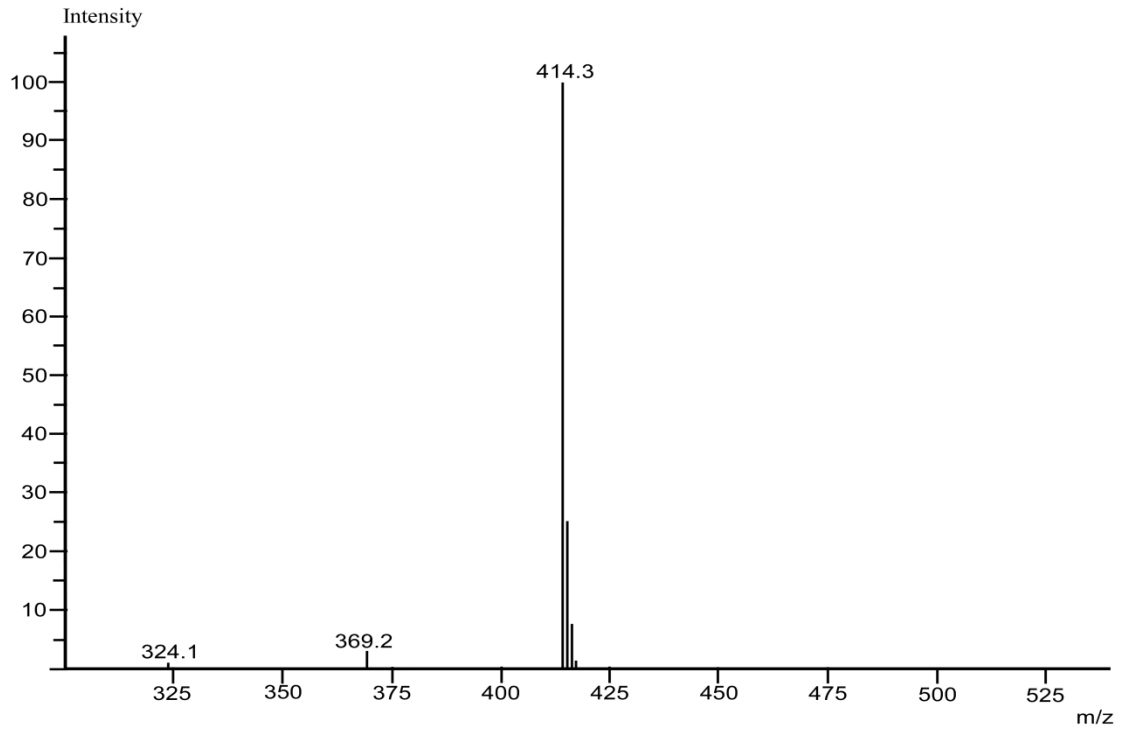


Fig. S6 ESI-MS of **3b** in DMSO-d<sub>6</sub>.

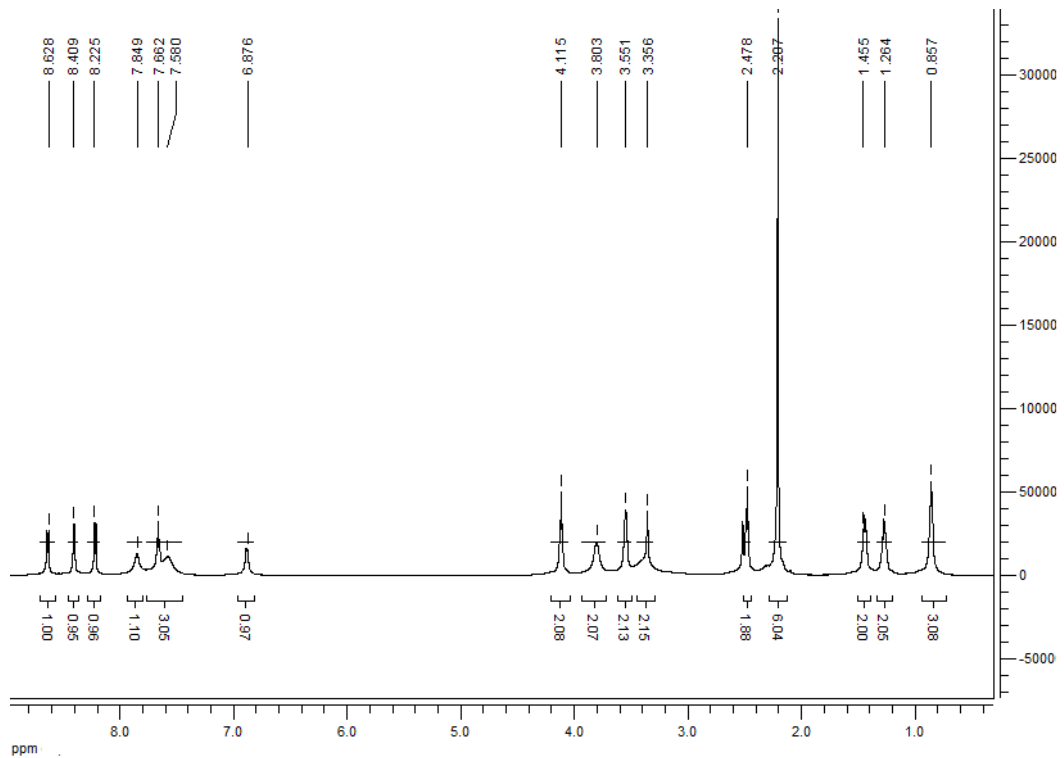
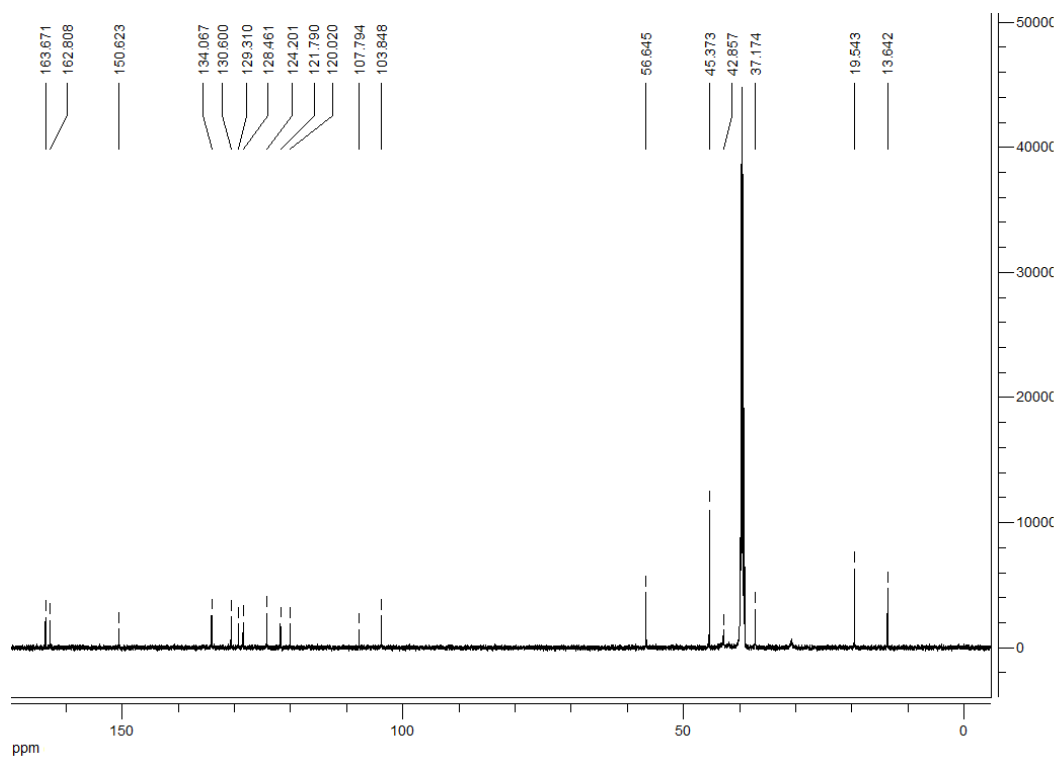


Fig. S7 <sup>1</sup>H NMR of **3c** in DMSO-d<sub>6</sub>.

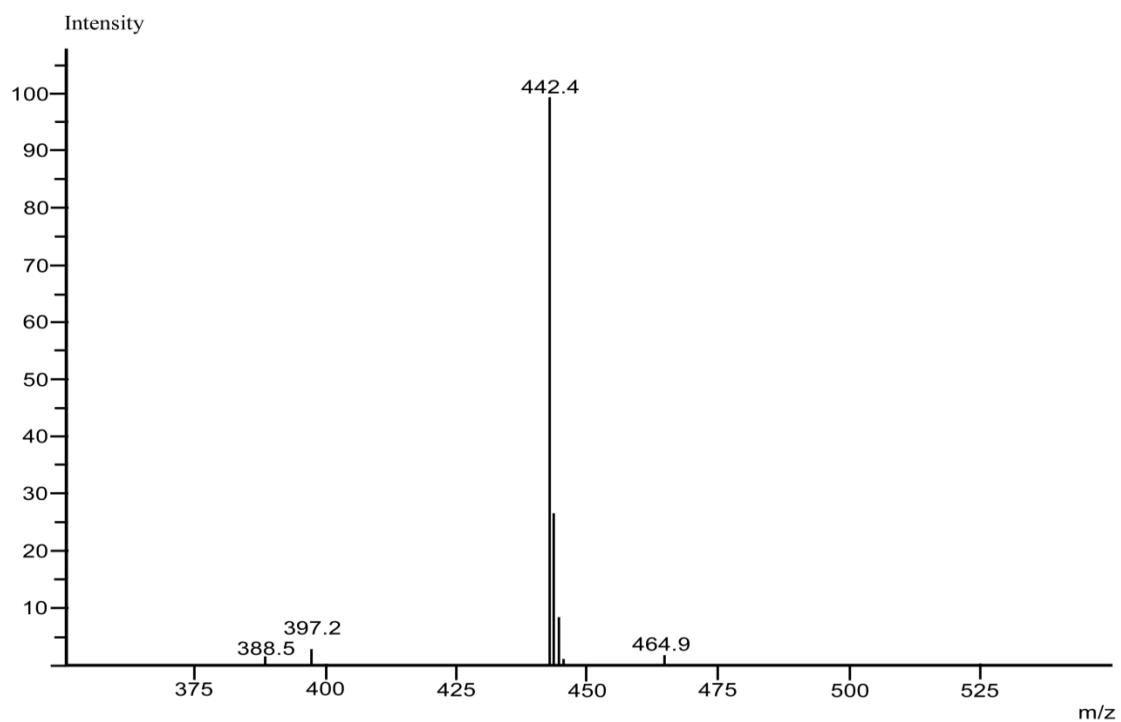


**Fig. S8**  $^{13}\text{C}$  NMR of **3c** in  $\text{DMSO-d}_6$ .

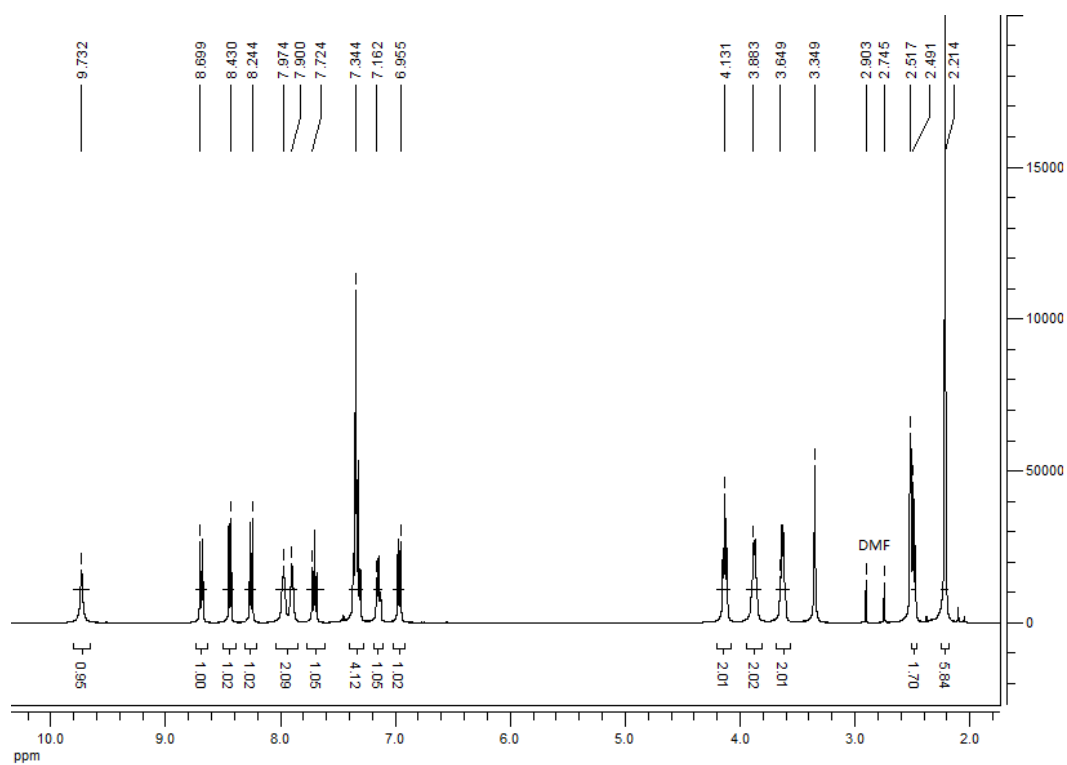
ESI-MS Spectrum, NIE-Bu

#:1 Ret Time:Averaged 1.333-1.653(Scan#:51-63)

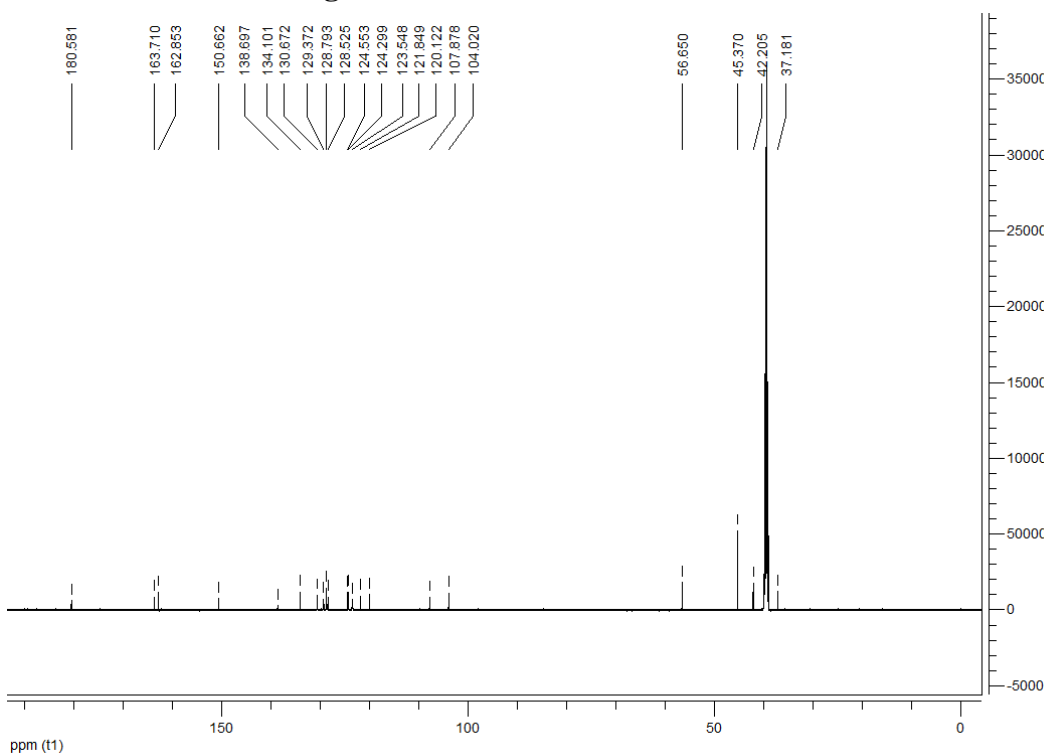
Mass Peaks:264 Base peak:442.35(1734737) Polarity:Pos Segment - Event1



**Fig. S9** ESI-MS of **3c** in  $\text{DMSO-d}_6$ .



**Fig. S10**  $^1\text{H}$  NMR of **3d** in  $\text{DMSO-d}_6$ .

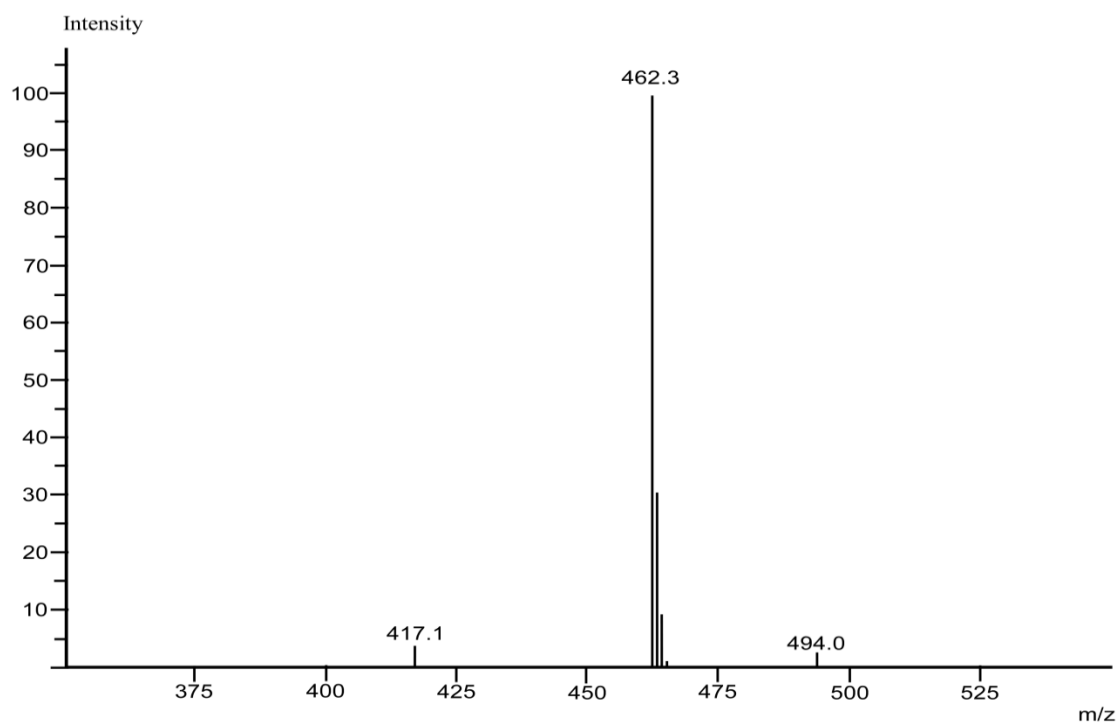


**Fig. S11**  $^{13}\text{C}$  NMR of **3d** in  $\text{DMSO-d}_6$ .

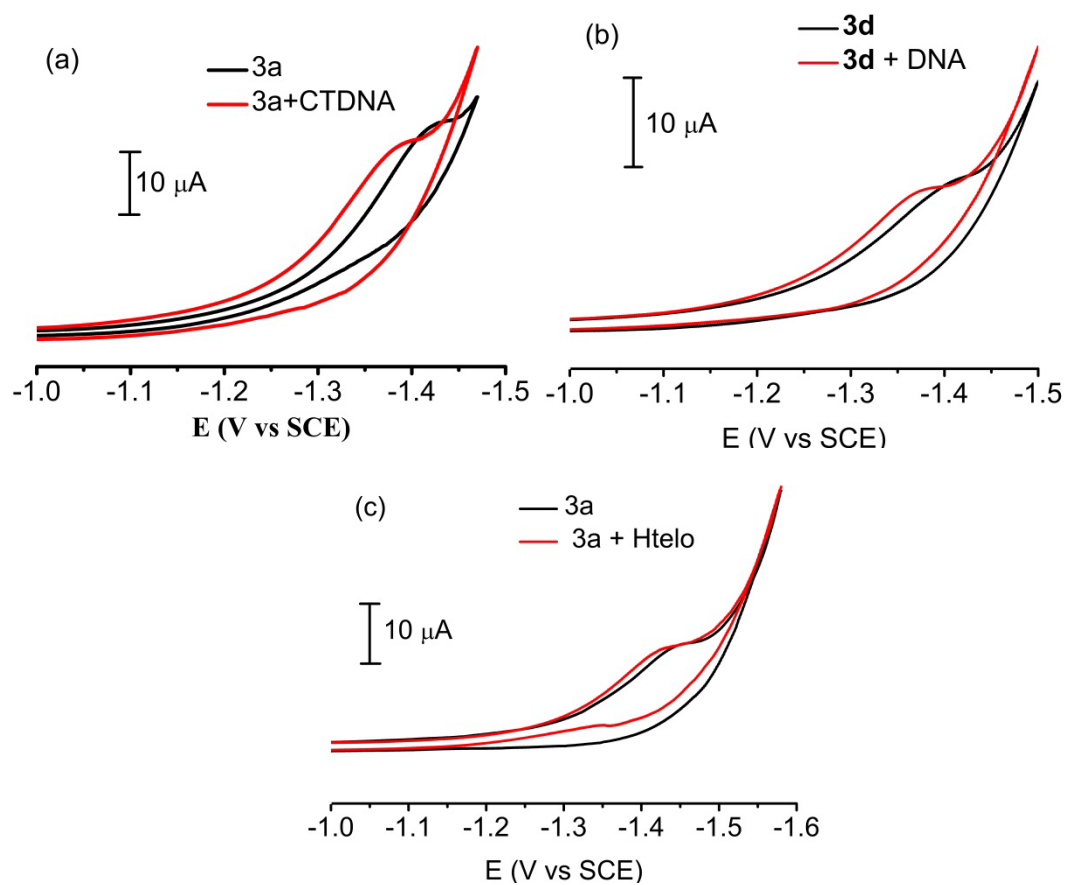
ESI-MS Spectrum,NIE-Ph

#:1 Ret Time:Averaged 1.360-1.627(Scan#:52-62)

Mass Peaks:226 Base peak:462.30(2082052) Polarity:Pos Segment - Event1

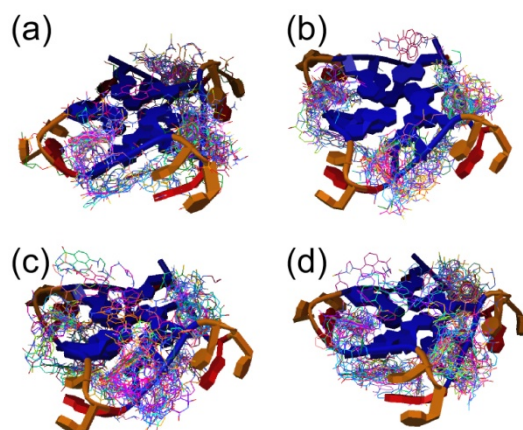


**Fig. S12** ESI-MS of **3d** in DMSO-d<sub>6</sub>.

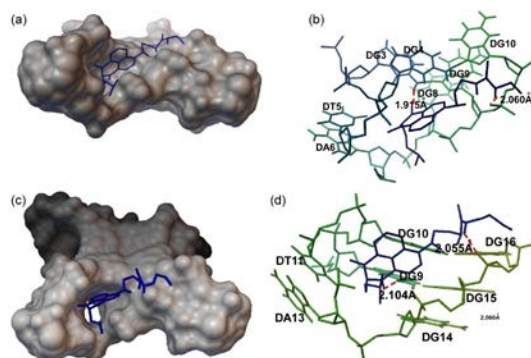


**Fig. S13** Cyclic voltammograms of (a) **3a** (50  $\mu\text{M}$ ) and (b) **3d** (50  $\mu\text{M}$ ) in the absence and presence of CT DNA (50  $\mu\text{M}$ ), and (c) **3a** (50  $\mu\text{M}$ ) in the absence and presence of Htelo G-quaruplex DNA (5  $\mu\text{M}$ ) in HEPES (10 mM, pH 7.4) buffer containing 0.1 M KCl. Scan rate 20  $\text{mV}\cdot\text{S}^{-1}$ .

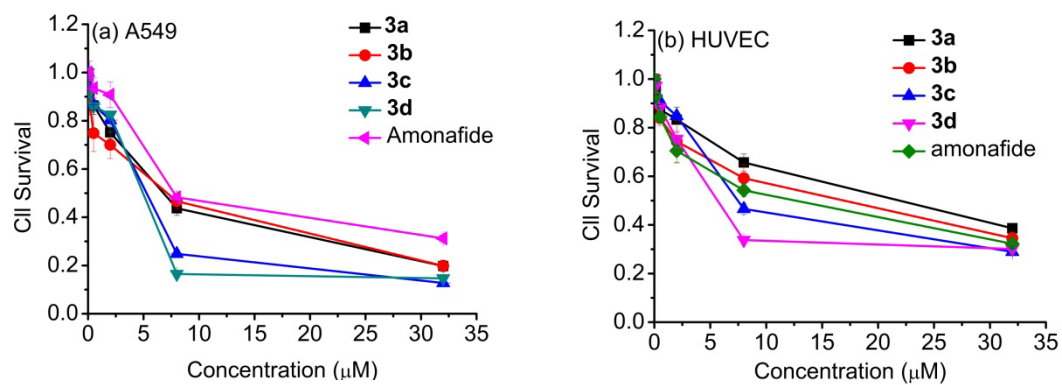




**Fig. S14** The docking results of platinum complexes (a) **1**, (b) **2** and (c) **3** in the different sites of telomeric G-quadruplex (PDB code: 1KF1).



**Fig. S15** Molecular docking Different views of the docked model of **3b** (a, b), **3c** (c, d) with telomeric G-quadruplex (PDB code: 1KF1). The red dotted line represents the lengths of the hydrogen bond.



**Fig. S16** Cytotoxicity of **3a-3d** and amonafide against (a) A549 and (b) HUVEC cells