- SUPPLEMENTARY MATERIAL -

Compound characterization

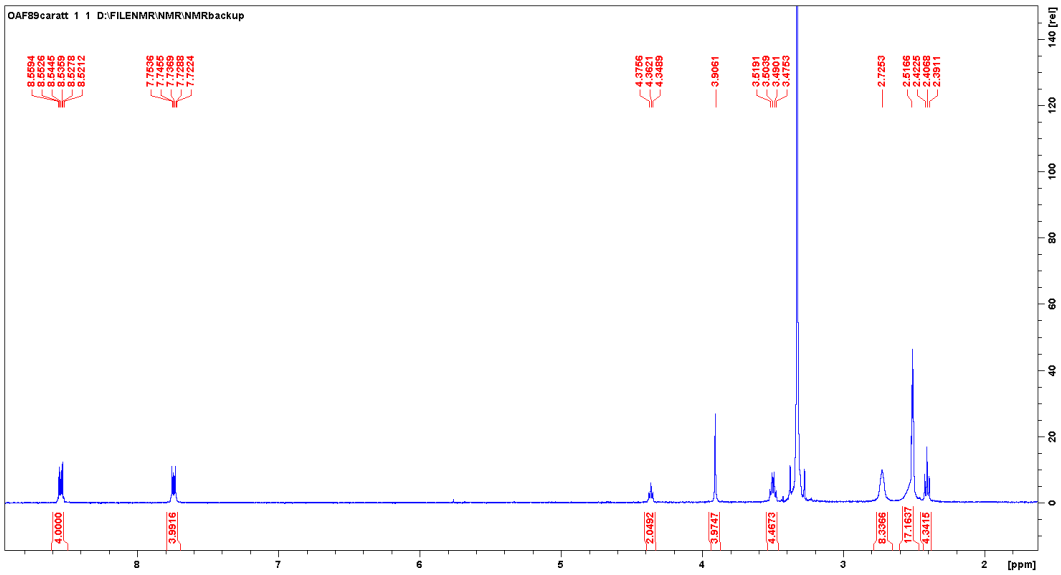

Figure S1. ^{1}H-NMR spectrum of compound **4**. Note: the signal of 4 x CH_2 protons (piperazine, bs) partially overlap with the signal of the solvent (DMSO-d_6).

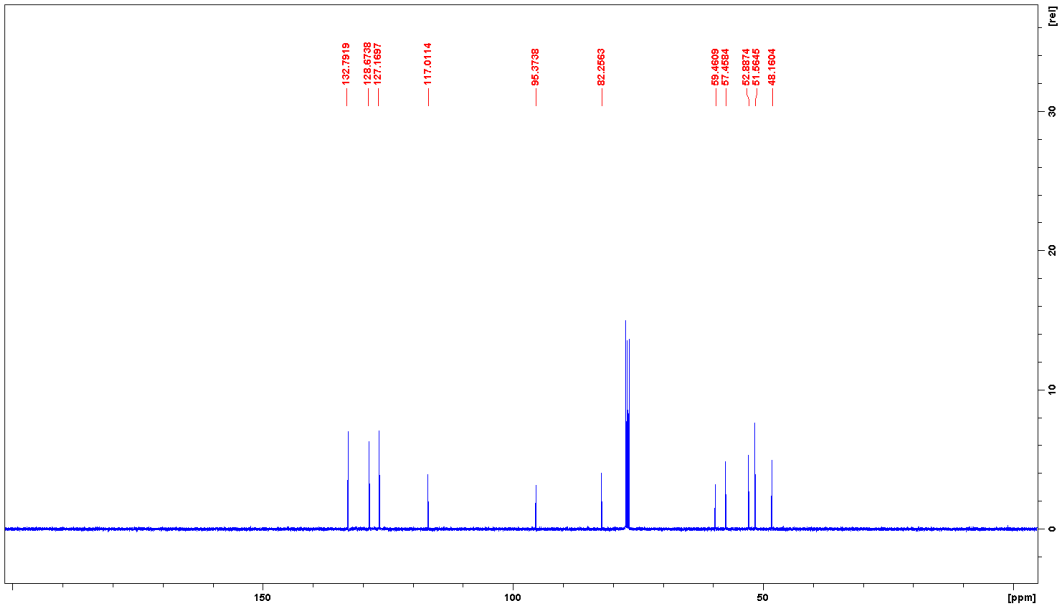

Figure S2. ^{13}C-NMR spectrum of compound **4** (DMSO-d_6).

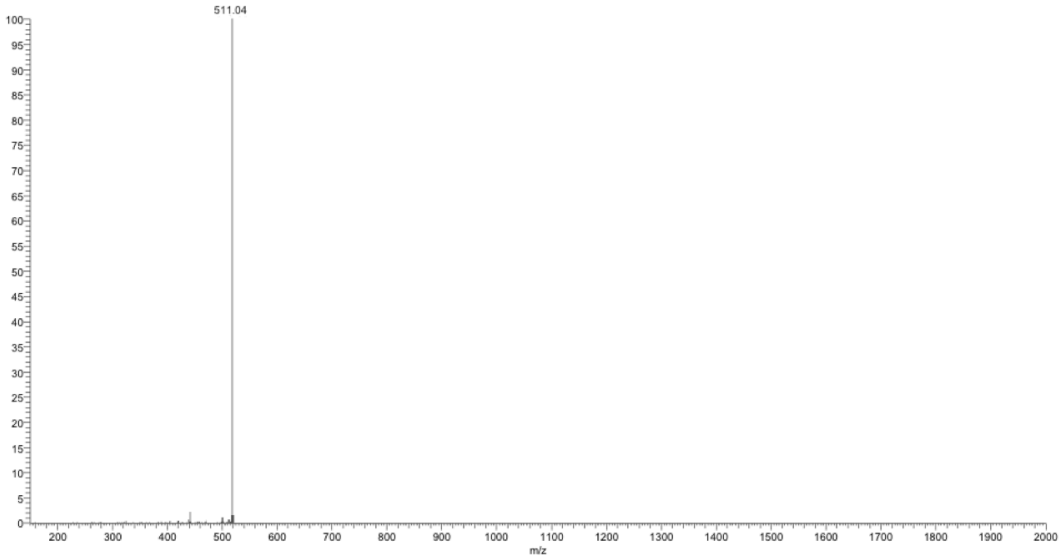

Figure S3. ESI-MS of compound **4** (positive ionization mode).

ESI-MS binding studies

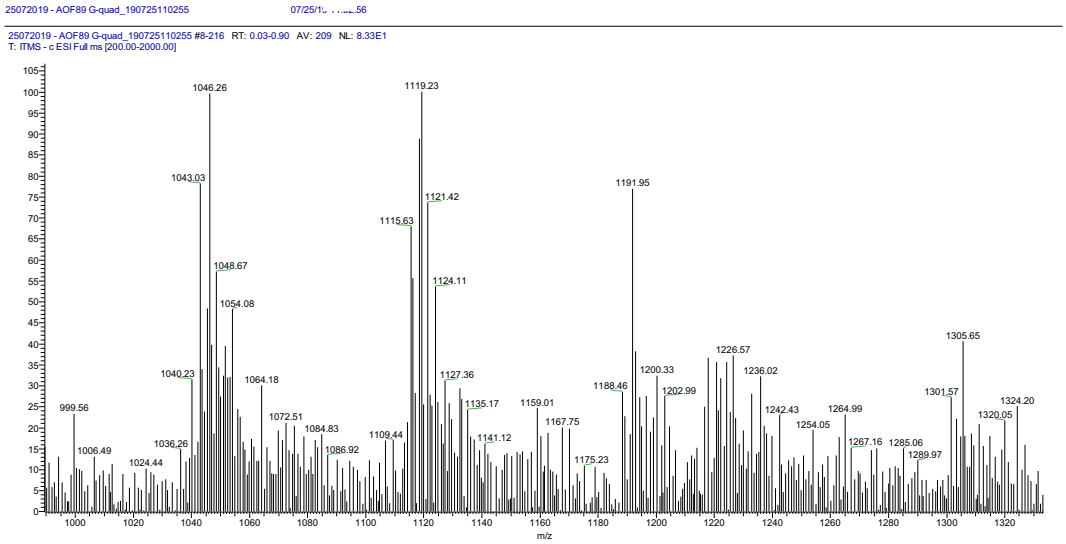

Figure S4. ESI-MS binding experiment of compound **4** with G-quadruplex DNA. Unbound G.quadruplex DNA (m/z = 1046.26, z = -7), ligand/G-quadruplex complex with 1:1 stoichiometry (m/z = 1119.23, z = -7) and ligand/G-quadruplex complex with 2:1 stoichiometry (m/z = 1191.95, z = -7) were detected.

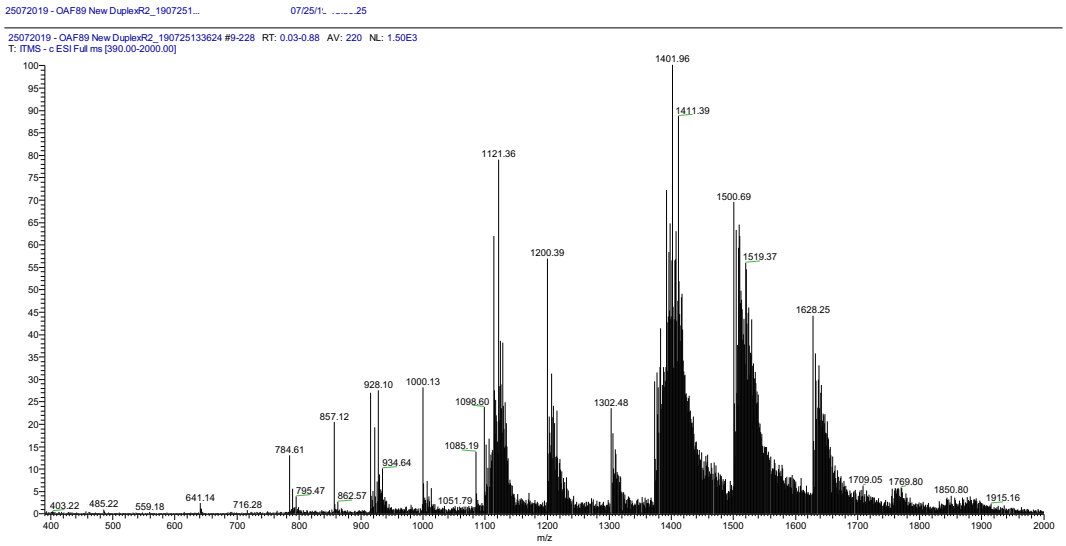

Figure S5. ESI-MS binding experiment of compound **4** with double-stranded DNA. Unbound dsDNA (m/z = 1121.36, z = -9), ligand/dsDNA complex with 1:1 stoichiometry (m/z = 1200.39, z = -9) and ligand/dsDNA complex with 2:1 stoichiometry (m/z = 1302.48, z = -9) were detected. The same behavior was observed in the z = -8 charge state.

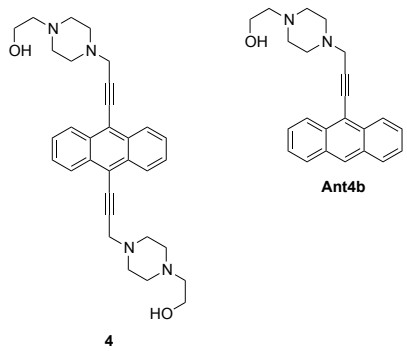

Figure S6. Chemical structures of compound **4** and of the monosubstituted analogue **Ant4b**.

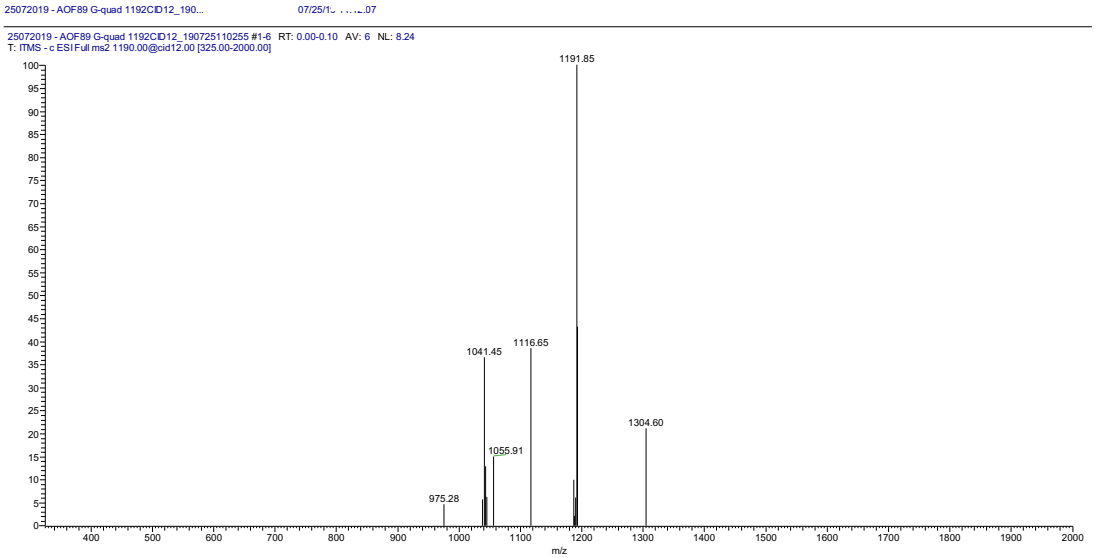

Figure S7. CID fragmentation spectrum of the ligand/G-quadruplex complex with 2:1 stoichiometry (normalized collision energy = 12). The fragmentation of the 2:1 ligand/G-quadruplex complex (m/z = 1191.85, z = -7) promoted the formation of the peaks corresponding to the 1:1 complex (m/z = 1116.65, z = -7) and to the unbound DNA (m/z = 1041.45, z = -7). Please note that the difference in m/z value for fragmentation peaks with respect to Figure S4 is due to instrumental resolution.

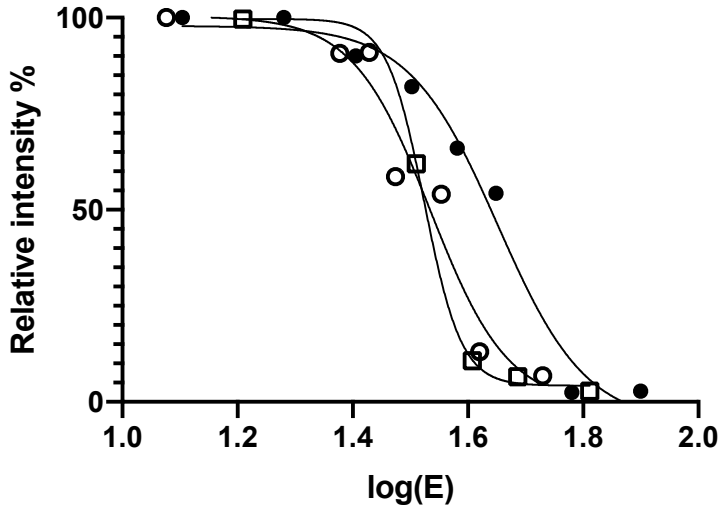

Figure S8. CID dissociation curves of the complexes. Black dots: ligand/G-quadruplex complex with 2:1 stoichiometry, white dots: ligand/G-quadruplex complex with 1:1 stoichiometry, white squares: ligand/dsDNA complex with 2:1 stoichiometry.