## $\dagger$ Electronic Supplementary Information (ESI)

## Experimental Section

## General procedure for synthesis of $\mathrm{Pt}(\mathrm{IV}) \mathrm{Cl}_{4}(\mathrm{BADs})_{2}$ complexes

Initially, the $\mathrm{K}_{2} \mathrm{PtCl}_{4}$ and BADs (molar ratio 1:2 respectively) were separately dissolved in freshly prepared solvent (absolute ethanol and Milli-Q water in 4:6 ratios respectively) using 1 MLH magnetic stirrer, REMI. Then the BADs solution was added drop wise in $\mathrm{K}_{2} \mathrm{PtCl}_{4}$ solution with a continuous stirring at room temperature. After 10 h , the mixture turned from light red brown into yellow and after 24 h , a yellow precipitate was formed on a completion of reaction. The ppt was filtered off, washed several times with water and ethanol, and was kept overnight in vacuum oven at room temperature for absolute dryness.

Table 1. Absorption at 240 nm for MBA, M2CBA, M3CBA, M4CBA and at 245 nm for M4FBA before and after DNA binding.

|  | MBA |  | M2CBA |  | M3CBA |  | M4CBA |  | M4FBA |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Conc. /M | Before | After | Before | After | Before | After | Before | After | Before | After |
| $1 \times 10^{-5}$ | 0.352 | 0 | 0.231 | 0 | 0.245 | 0 | 0.291 | 0 | 0.200 | 0 |
| $3 \times 10^{-5}$ | 0.621 | 0 | 0.651 | 0 | 0.520 | 0 | 0.659 | 0 | 0.290 | 0 |
| $5 \times 10^{-5}$ | 0.820 | 0 | 0.819 | 0 | 0.766 | 0 | 0.942 | 0 | 0.368 | 0.037 |
| $7 \times 10^{-5}$ | 1.109 | 0 | 0.926 | 0.385 | 0.924 | 0.055 | 1.109 | 0 | 0.510 | 0.135 |
| $9 \times 10^{-5}$ | 1.396 | 0.421 | 1.033 | 0.458 | 1.201 | 0.327 | 1.240 | 0.216 | 0.809 | 0.224 |



Fig. 1 Absorption spectra of DNA ( $5 \times 10-5 \mathrm{M}$ ) in absence and presence of increasing amounts of MBA (ri = [complex]/[DNA]).


Fig. 2 Absorption spectra of DNA ( $5 \times 10^{-5} \mathrm{M}$ ) in absence and presence of increasing amounts of M2CBA (ri = [complex]/[DNA]).


Fig. 3 Absorption spectra of DNA $\left(5 \times 10^{-5} \mathrm{M}\right)$ in absence and presence of increasing amounts of M3CBA (ri = [complex]/[DNA]).


Fig. 4 Absorption spectra of DNA $\left(5 \times 10^{-5} \mathrm{M}\right)$ in absence and presence of increasing amounts of M4CBA (ri = [complex]/[DNA]).


Fig. 5 Absorption spectra of DNA $\left(5 \times 10^{-5} \mathrm{M}\right)$ in absence and presence of increasing amounts of M4CBA (ri = [complex]/[DNA]).


Fig. 6 Absorption spectra of DNA $\left(5 \times 10^{-5} \mathrm{M}\right)$ in absence and presence of increasing amounts of ligand phenylmethanamine (ri = [phenylmethanamine]/[DNA]).


Fig. 7 Drug-Friccohesity Interaction model which support to anticancer activity of drug.

