

Supporting Information

Evaluation of *O*-Alkyl and Aryl Sulfonyl Aromatic and Heteroaromatic Amidoximes as Novel Potent DNA Photo-cleavers

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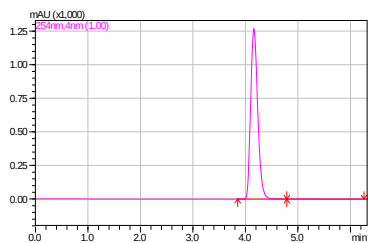
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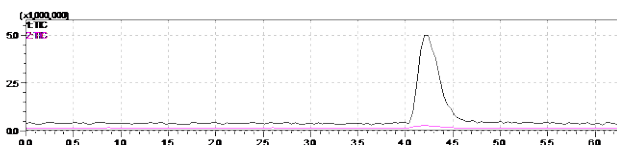
Photochemistry

LC-MS analysis of compound 19

UV detection

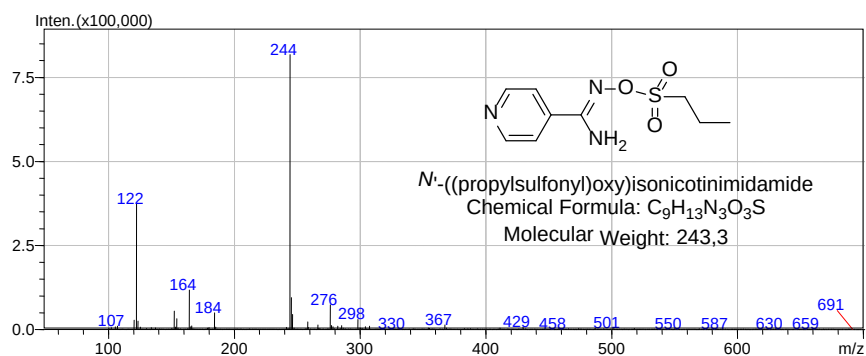


MS detection

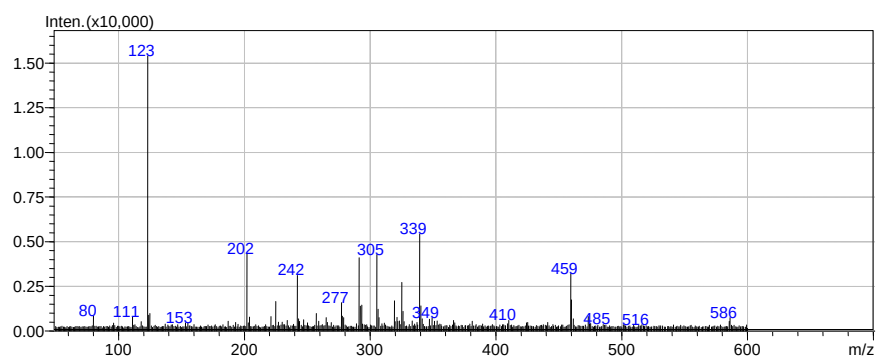


Time = 4-4.5 min

Positive spectrum

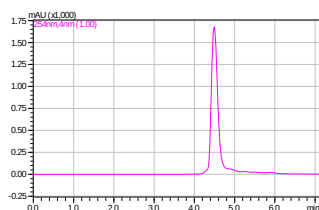


Negative spectrum

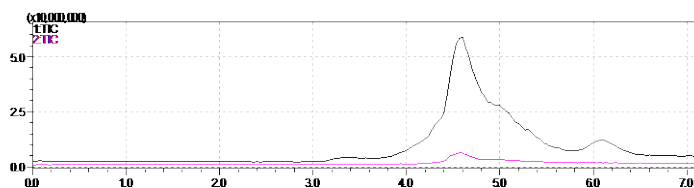


LC-MS analysis of photochemical degradation of compound 19 in benzene

UV detection

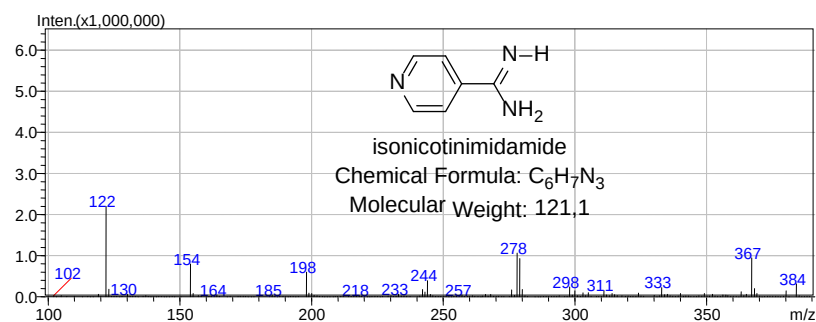


MS detection



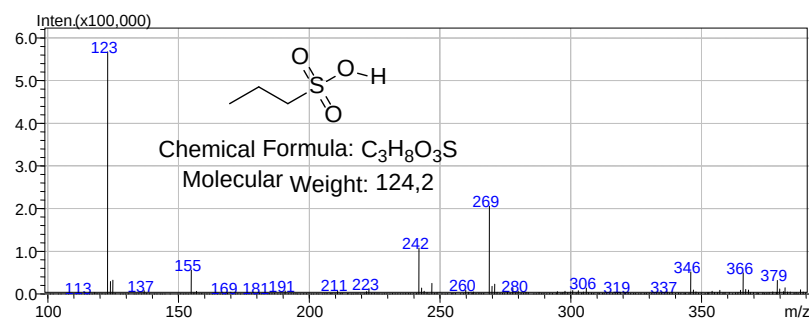
Time = 4.3-5.3 min

Positive spectrum



122 [isonicotinimidamide+H]⁺, 154 [isonicotinimidamide+H+MeOH]⁺.

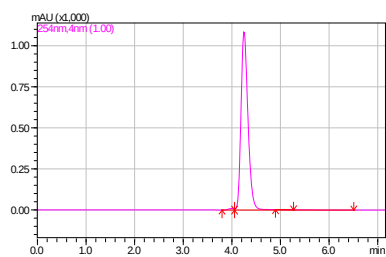
Negative spectrum



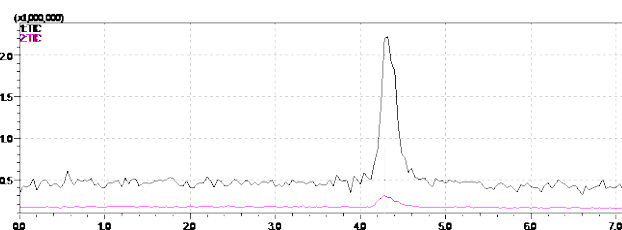
123 [propyl sulfonic acid-H]⁻.

LC-MS analysis of compound 24

UV detection

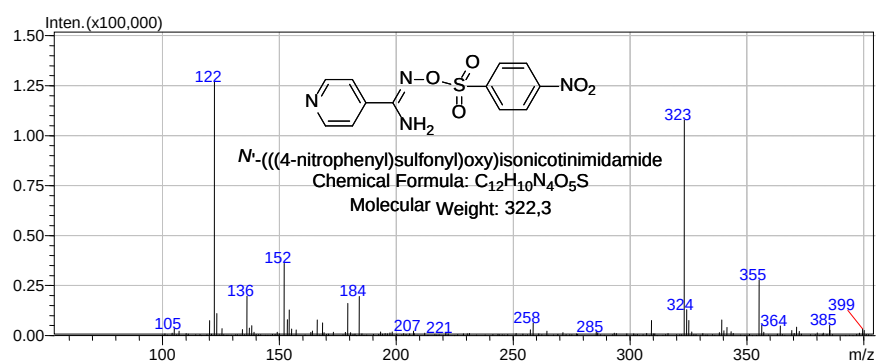


MS detection

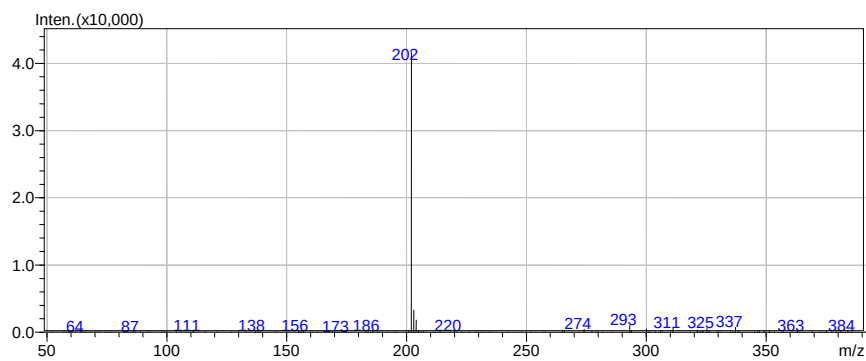


Time = 4.1-4.5 min

Positive spectrum

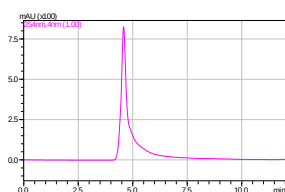


Negative spectrum

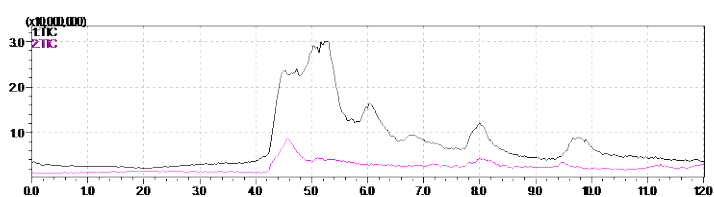


LC-MS analysis of photochemical degradation of compound 24 in MeOH/H₂O

UV detection

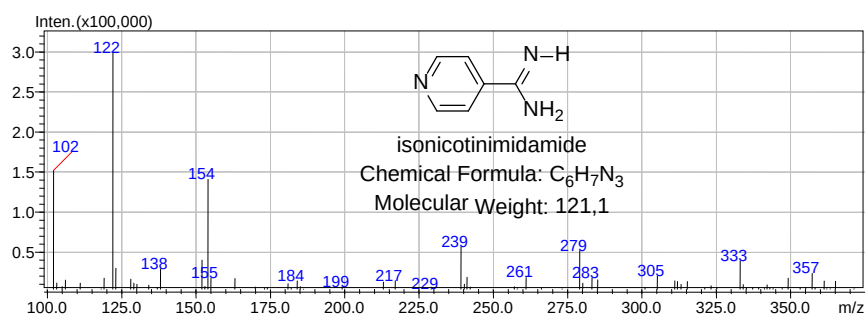


MS detection



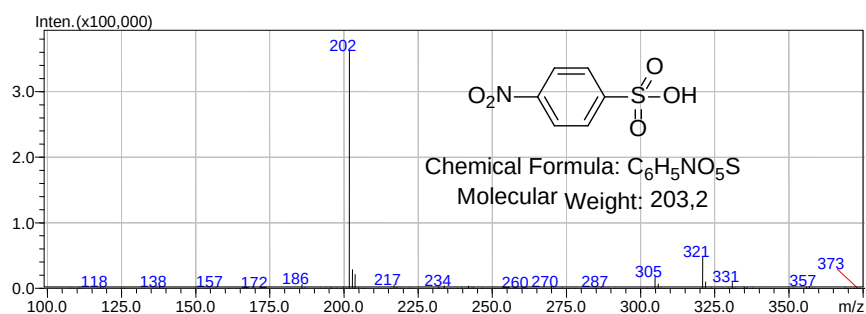
Time = 4.1-10.2 min

Positive spectrum



122 [isonicotinimidamide+H]⁺, 154 [isonicotinimidamide+H+MeOH]⁺.

Negative spectrum



202 [p-nitro-phenyl sulfonic acid-H]⁻.

Molecular Biology

Dose measurement gel electrophoresis for compounds **6**, **12** and **24**.

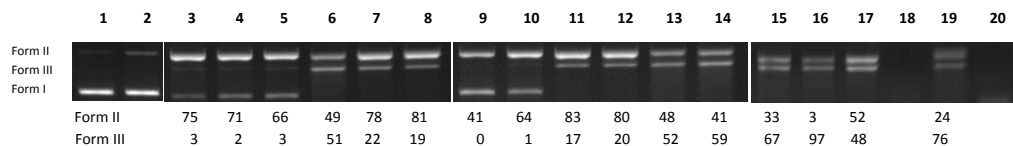


Figure S1. Top: Dose measurement gel electrophoresis data for the irradiation of compounds **6**, **12** and **24** (500-1000 μ M). Lane 1: DNA without UV irradiation; Lane 2: DNA with UV irradiation; Lane 3: DNA + **6** (500 μ M); Lane 4: DNA + **6** (600 μ M); Lane 5: DNA + **6** (700 μ M); Lane 6: DNA + **6** (800 μ M); Lane 7: DNA + **6** (900 μ M); Lane 8: DNA + **6** (1000 μ M); Lane 9: DNA + **12** (500 μ M); Lane 10: DNA + **12** (600 μ M); Lane 11: DNA + **12** (700 μ M); Lane 12: DNA + **12** (800 μ M); Lane 13: DNA + **12** (900 μ M); Lane 14: DNA + **12** (1000 μ M); Lane 15: DNA + **25** (500 μ M); Lane 16: DNA + **24** (600 μ M); Lane 17: DNA + **24** (700 μ M); Lane 18: DNA + **24** (800 μ M); Lane 19: DNA + **24** (900 μ M); Lane 20: DNA + **24** (1000 μ M); Bottom: Calculation of the % conversion to ss and ds. § When the compound is very active the plasmid is broken in many pieces and cannot be seen on the gel.

Gel electrophoresis: mechanistic studies for compound **24**.

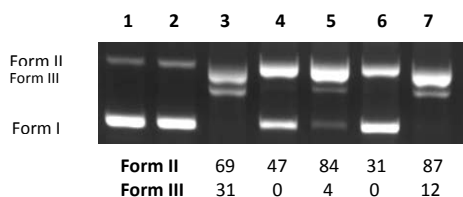


Figure S2. Top: Gel electrophoresis data. Mechanistic studies involved at the DNA cleavage upon irradiation by derivative **24** (500 μ M). Lane 1: DNA without UV irradiation; Lane 2: DNA with UV irradiation; Lane 3: DNA + **24**; Lane 4: DNA + **24** + argon; Lane 5: DNA + **24** + DMSO (20%); Lane 6: DNA + **24** + NaN_3 ; Lane 7: DNA + **24** + D_2O ; Bottom: Calculation of the % conversion to ss and ds.

Gel electrophoresis for compound **16** in various pH.

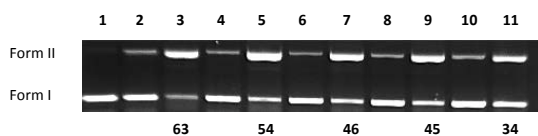


Figure S3. Top: Gel electrophoresis data of compound **16** (800 μ M) upon irradiation in various pH. Lane 1: DNA without UV irradiation; Lane 2: DNA with UV irradiation at pH 5; Lane 3: DNA + **16** at pH 5; Lane 4: DNA with UV irradiation at pH 6; Lane 5: DNA + **16** at pH 6; Lane 6: DNA with UV irradiation at pH 7; Lane 7: DNA + **16** at pH 7; Lane 8: DNA with UV irradiation at pH 8; Lane 9: DNA + **16** at pH 8; Lane 10: DNA with UV irradiation at pH 9; Lane 11: DNA + **16** at pH 9; Bottom: Calculation of the % conversion to ss damage.

DNA affinity calculations

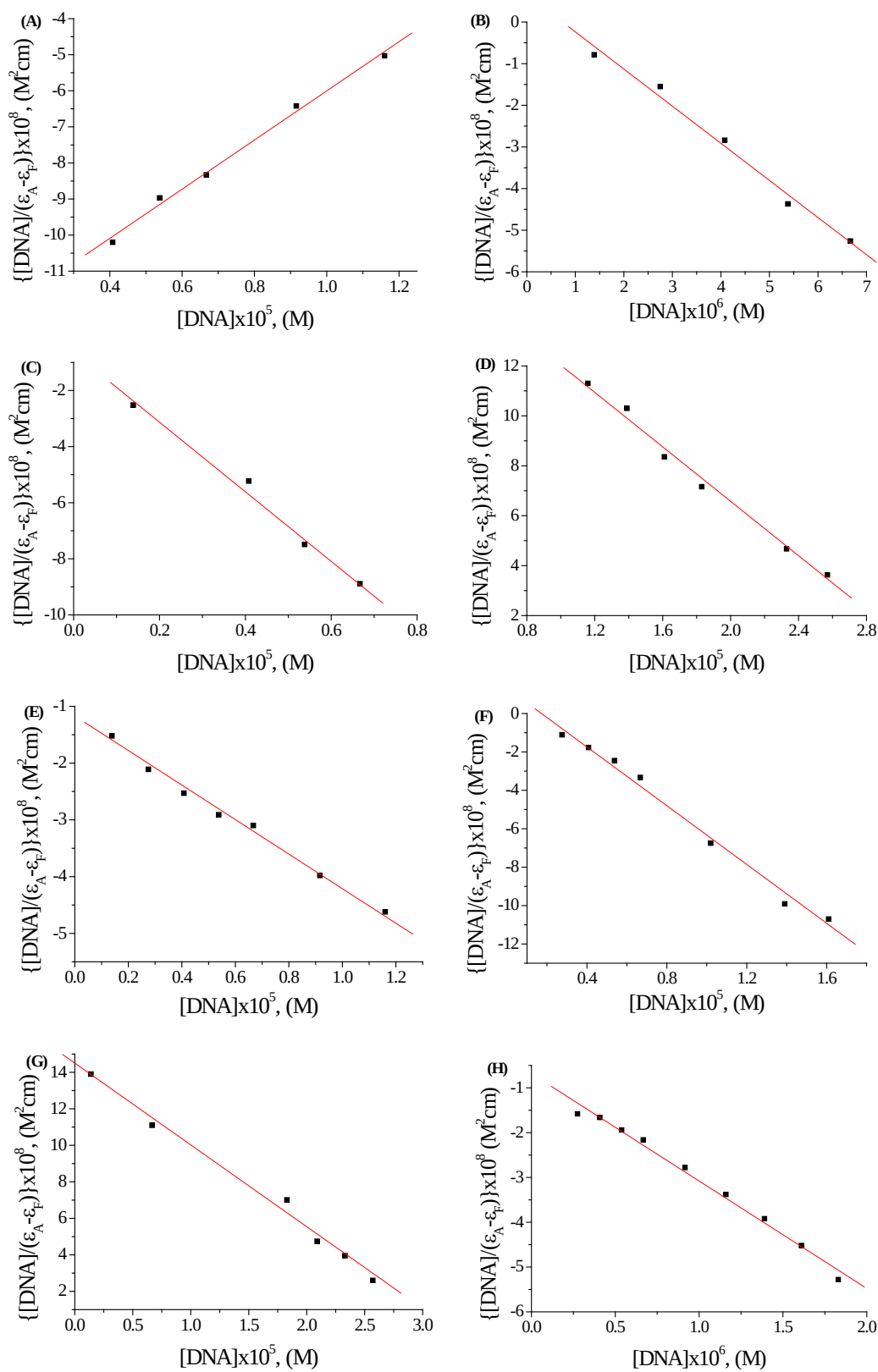


Figure S4. Plot of $\frac{[DNA]}{(\epsilon_A - \epsilon_f)}$ vs $[DNA]$ for compound (A) **6**, (B) **18**, (C) **19**, (D) **20**, (E) **21**, (F) **22**, (G) **23** and (H) **24**.

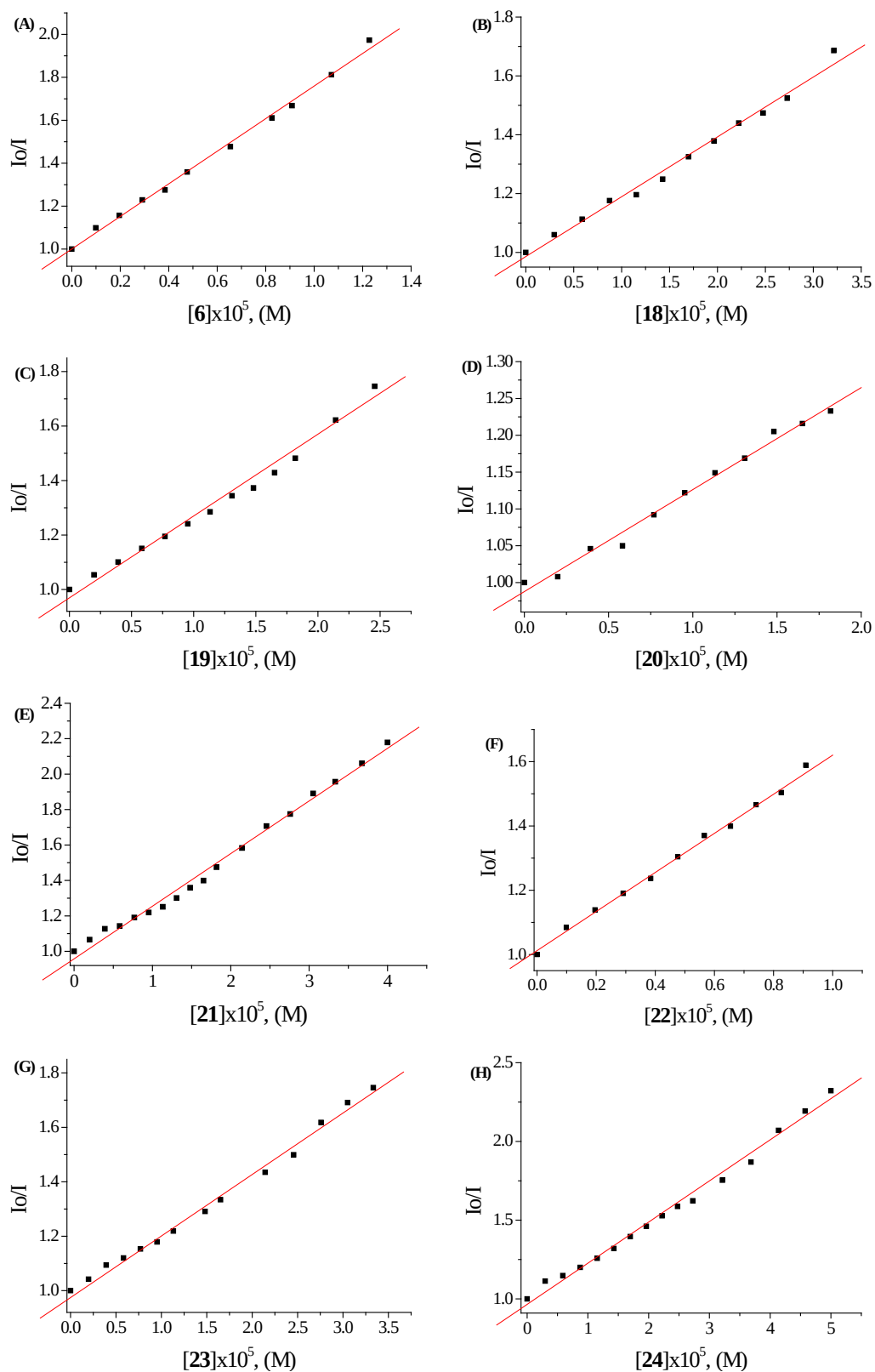


Figure S5. Stern–Volmer quenching plot of EB bound to CT DNA for compound (A) 6, (B) 18, (C) 19, (D) 20, (E) 21, (F) 22, (G) 23 and (H) 24.