

CHEMISTRY

A **European** Journal

Supporting Information

DNA Oxidation Photoinduced by Norharmane Rhenium(I) Polypyridyl Complexes: Effect of the Bidentate N,N'-Ligands on the Damage Profile

Iván Maisuls,^[a, b] Franco M. Cabrerizo,^{*[a]} Pedro M. David-Gara,^[c] Bernd Epe,^[d] and Gustavo T. Ruiz^{*[b]}

chem_201801272_sm_miscellaneous_information.pdf

Supplementary Information

DNA oxidation photoinduced by Norharmane Rhenium(I) polypyridyl complexes: effect of the bidentate N,N' ligands on the damage profile

Iván Maisuls^{[a][b]}, Franco M. Cabrerizo^{[a]*}, Pedro M. David-Gara^[c], Bernd Epe^[d] and Gustavo T. Ruiz^{[b]*}

[a] I. Maisuls, Dr. F. M. Cabrerizo

Instituto de Investigaciones Biotecnológicas – Instituto de Tecnología Chascomus (IIB – INTECH)

Universidad Nacional de San Martín (UNSAM)

I. Marino, Km 8.2 CC 164, (7130) Chascomus, Argentina.

E-mail: fcabrerizo@intech.gov.ar

[b] I. Maisuls, Dr. G. T. Ruiz

Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA)

Universidad Nacional de la Plata (UNLP), CCT La Plata-CONICET

Diag. 113 y 64, Sucursal 4, C.C. 16, (B1906ZAA) La Plata, Argentina

E-mail: gruiz@inifta.unlp.edu.ar

[c] Dr. P.M. David-Gara

Centro de Investigaciones Ópticas (CIOP – CONICET – CIC)

Universidad Nacional de La Plata

C.C.3, (1897), La Plata. Argentina

[d] Dr. B. Epe

Institute of Pharmacy and Biochemistry

University of Mainz

Staudingerweg 5, D-55099 Mainz, Germany

Contents:		<u>Page</u>
1.	Dark controls	S3
2.	Normalized emission spectra of ReBpy , RePhen and ReDppz in different solvents	S4
3.	Laser Flash Photolysis of ReDppz in methanol and water	S5
4.	Fluorescence decays of the ${}^1L_{nH_0}$ band in ReBpy and RePhen	S6
5.	Mutants per millon survivors for RePhen	S7

1. Dark controls

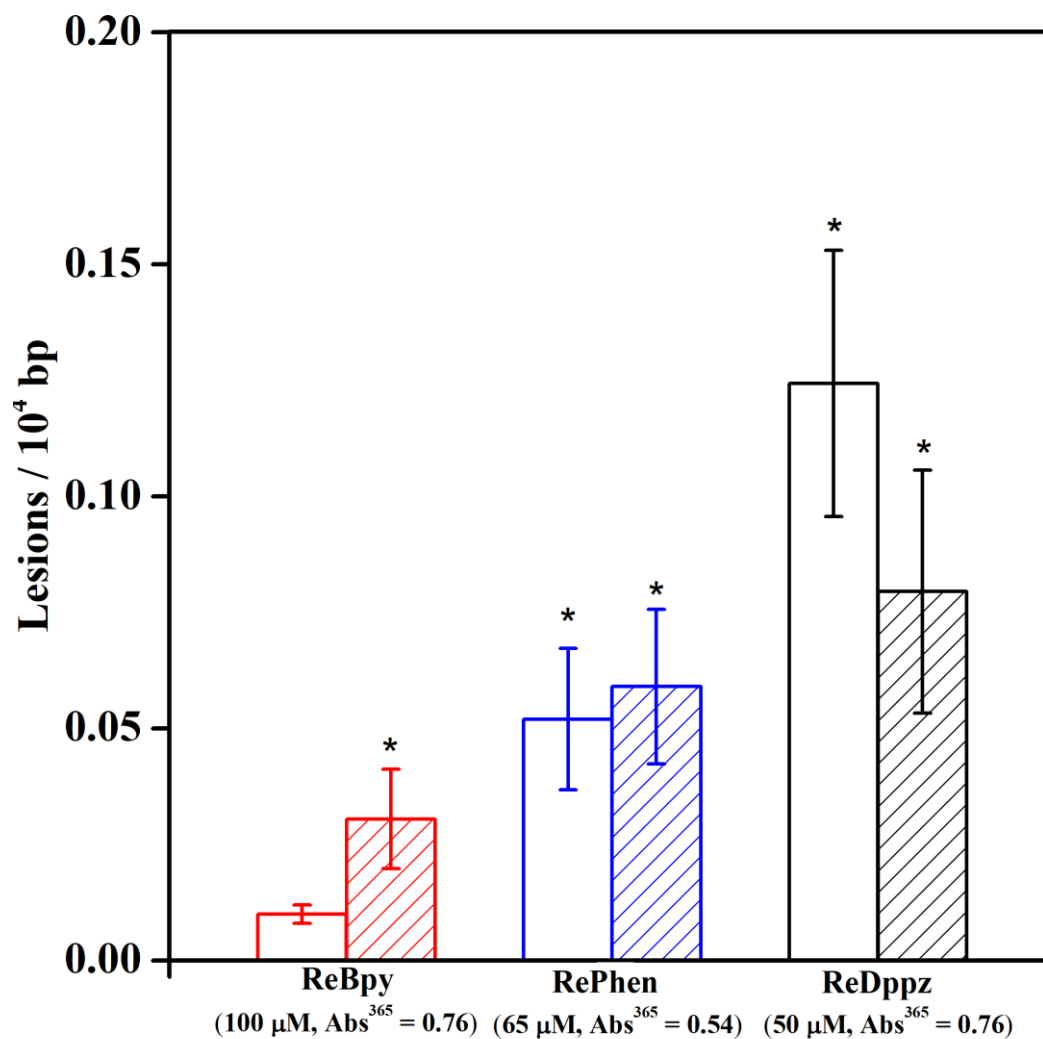


Figure SI.1. SSBs (empty bars) and Fpg-sensitive modifications (dashed bars) observed in PM2 DNA incubated with the maximum concentration of **ReBpy** (red), **RePhen** (blue) and **ReDppz** (black). All the experiments were performed in phosphate buffer solutions (pH 7.4) and data are the mean of 4 independent experiments (\pm S.D).

2. Normalized emission spectra of ReBpy, RePhen and ReDppz in different solvents

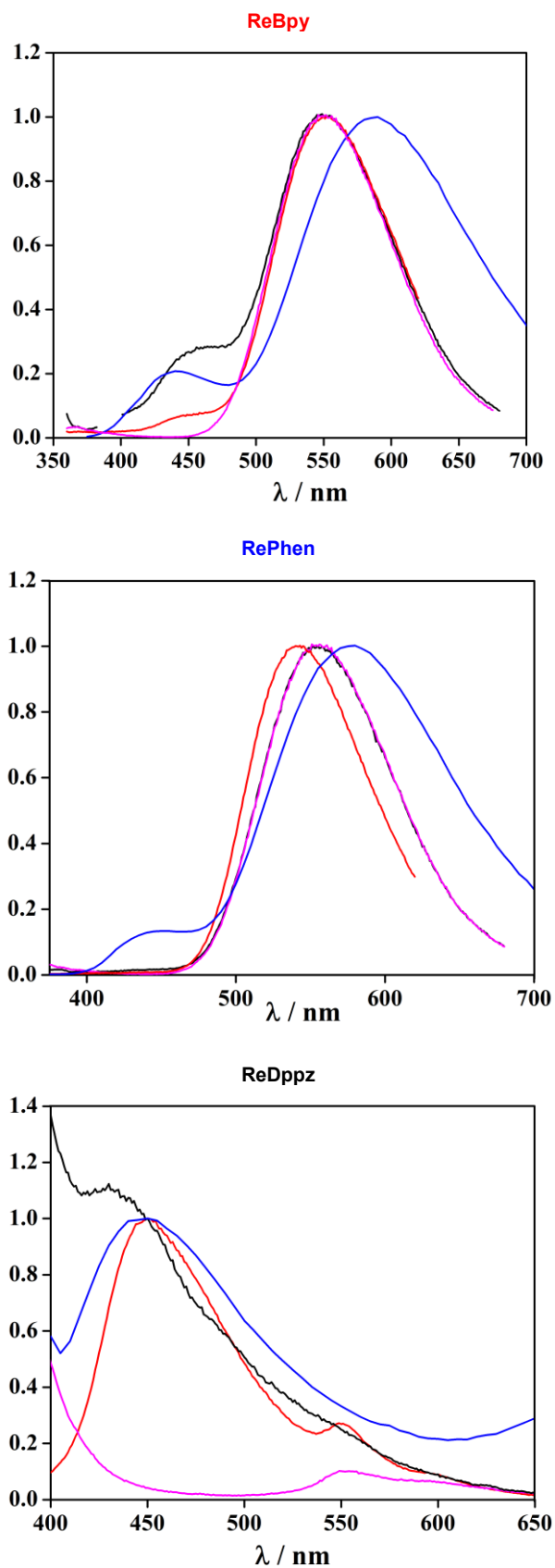


Figure S1.2. Normalized emission spectra of **ReBpy**, **RePhen** and **ReDppz** in: MeOH (*Black*), CH₂Cl₂ (*Red*), acetonitrile (*Magenta*) and phosphate buffer pH = 7.4 (*Blue*). In Acetonitrile the emission of the IL_{nlH₀} is shifted to $\lambda \approx 380$ nm (not shown), as seen in different low polar aprotic solvents.^[1]

3. Laser Flash Photolysis trace of ReDppz in methanol and water

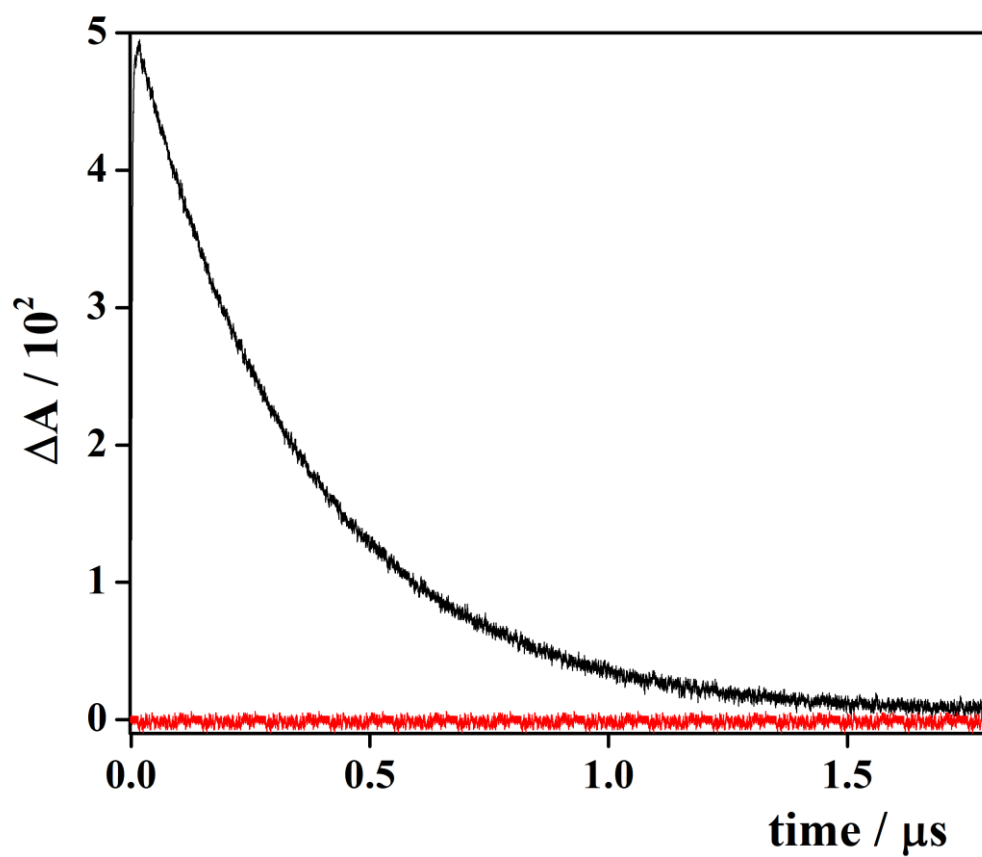


Figure S1.3. Laser Flash Photolysis of ReDppz in MeOH (Black) and in H₂O (Red). $\lambda_{\text{obs}} = 460 \text{ nm}$. [2]

4. Fluorescence decays of the IL_{nH_0} band for ReBpy and RePhen

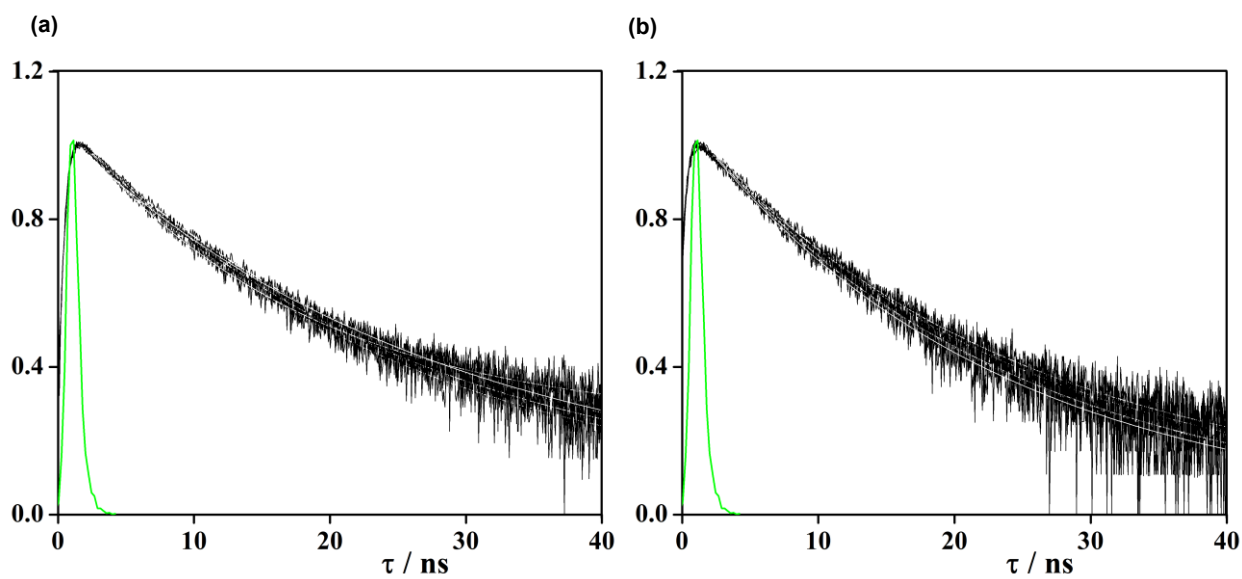


Figure SI.4. Fluorescence decays (black lines) recorded at wavelengths of the emission maximum of the corresponding IL_{nH_0} transition (450 nm) for **ReBpy** (a) and **RePhen** (b). $\lambda_{\text{exc}} = 341$ nm. Prompt signal and mono-exponential fitting curves are depicted as green and white lines, respectively.

5. Mutants per million survivors for RePhen

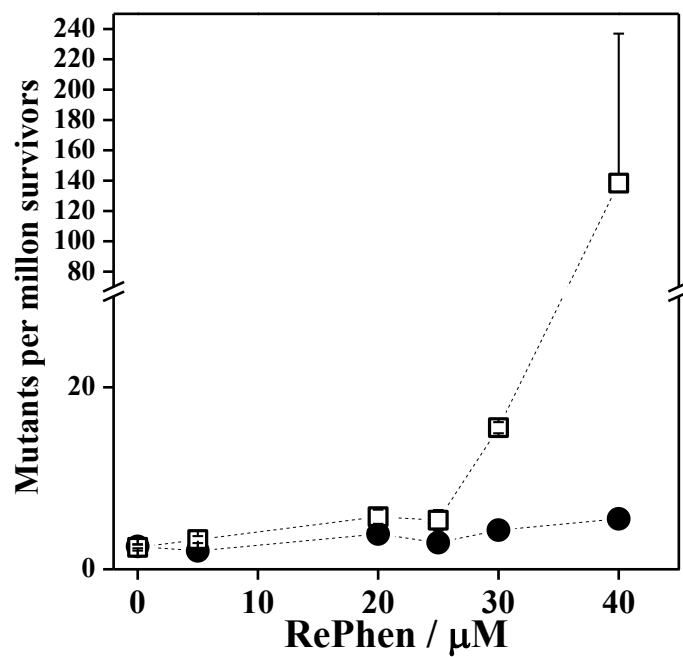


Figure SI.5. Mutations per million survivors for RePhen

[1] S. Draxler and L. M. E., *J. Phys. Chem.* **1993**, 97, 11493 - 11496.

[2] I. Maisuls, M. F. Cabrerizo, G. A. Lappin, G. T. Ruiz and J. G. Ferraudi, *J. Photochem. Photobiol.* **2018**, Submitted.