

Supplementary information for

Water Exchange Rates of Water-Soluble Manganese(III) Porphyrins of Therapeutical Potential

Ana Budimir,^a József Kalmár,^{b*} István Fábián,^b Gábor Lente,^b István Bánai,^c Ines Batinić-Haberle,^d and Mladen Biruš^{a*}

^a Faculty of Pharmacy and Biochemistry, University of Zagreb, Ante Kovačića 1, 10000 Zagreb, Croatia. E-mail: birus@pharma.hr

^b Department of Inorganic and Analytical Chemistry, University of Debrecen, Debrecen 10, POB 21, Hungary, H-4010. E-mail: jkalmar@dragon.unideb.hu

^c Department of Colloid and Environmental Chemistry, University of Debrecen, Hungary.

^d Duke University Medical School, Department of Radiation Oncology, Durham, NC 27710, USA

Mn^{III}TE-2-PyP⁵⁺

T (K)	1/T1 _{red} (1/s)	1/T2 _{red} (1/s)	delta _{red} (rad/s)
280	5.181.E+05	1.291.E+06	-4.309.E+05
285	5.190.E+05	1.563.E+06	-4.184.E+05
290	4.016.E+05	1.881.E+06	-7.756.E+05
295	2.616.E+05	2.400.E+06	-9.814.E+05
300	2.528.E+05	2.508.E+06	-1.372.E+06
305	2.522.E+05	2.941.E+06	-1.926.E+06
310	2.044.E+05	3.118.E+06	-2.050.E+06
315	1.737.E+05	2.997.E+06	-2.700.E+06
320	1.659.E+05	3.089.E+06	-3.104.E+06
325	1.851.E+05	2.925.E+06	-3.307.E+06
335	1.365.E+05	2.547.E+06	-3.661.E+06

MicroMath Scientist 2.0 Nonlinear Least-Squares Fit

280	4.972E+05	1.302E+06	-2.449E+05
285	4.586E+05	1.640E+06	-4.088E+05
290	4.057E+05	1.998E+06	-6.476E+05
295	3.495E+05	2.346E+06	-9.687E+05
300	2.966E+05	2.646E+06	-1.363E+06
305	2.499E+05	2.865E+06	-1.804E+06
310	2.100E+05	2.988E+06	-2.251E+06
315	1.766E+05	3.020E+06	-2.669E+06
320	1.489E+05	2.981E+06	-3.030E+06
325	1.259E+05	2.895E+06	-3.323E+06
335	9.106E+04	2.663E+06	-3.717E+06

Mn^{III}TnHex-2-PyP⁵⁺

T (K)	1/T1_{red} (1/s)	1/T2_{red} (1/s)	delta_{red} (rad/s)
283	6.804E+05	2.196E+06	-1.198E+06
288	5.526E+05	2.449E+06	-1.315E+06
293	6.308E+05	3.171E+06	-1.605E+06
297	6.031E+05	3.540E+06	-1.710E+06
300	5.113E+05	3.914E+06	-2.325E+06
305	5.130E+05	4.451E+06	-2.496E+06
310	4.839E+05	4.743E+06	-3.045E+06
315	4.194E+05	5.165E+06	-3.597E+06
320	4.016E+05	5.111E+06	-4.445E+06
325	3.950E+05	5.362E+06	-5.043E+06
330	3.324E+05	5.271E+06	-5.343E+06
335	3.047E+05	5.042E+06	-5.349E+06

MicroMath Scientist 2.0 Nonlinear Least-Squares Fit

283	6.469E+05	2.311E+06	-5.598E+05
288	6.276E+05	2.829E+06	-8.708E+05
293	5.974E+05	3.357E+06	-1.288E+06
297	5.688E+05	3.759E+06	-1.694E+06
300	5.461E+05	4.034E+06	-2.034E+06
305	5.077E+05	4.424E+06	-2.640E+06
310	4.700E+05	4.718E+06	-3.258E+06
315	4.342E+05	4.921E+06	-3.844E+06
320	4.009E+05	5.054E+06	-4.368E+06
325	3.702E+05	5.143E+06	-4.815E+06
330	3.422E+05	5.210E+06	-5.183E+06
335	3.166E+05	5.271E+06	-5.477E+06



T (K)	1/T1 _{red} (Hz)	1/T2 _{red} (Hz)	delta _{red} (rad/s)
275	6.121E+05	2.539E+06	-1.139E+06
280	2.413E+05	3.679E+06	-1.959E+06
285	1.247E+05	4.241E+06	-3.088E+06
290	1.657E+05	4.572E+06	-3.827E+06
295	3.296E+05	4.223E+06	-4.595E+06
300	2.573E+05	4.370E+06	-5.382E+06
305	2.542E+05	4.095E+06	-5.553E+06
310	2.577E+05	3.604E+06	-5.825E+06
315	2.492E+05	3.448E+06	-6.208E+06
320	2.192E+05	3.251E+06	-6.081E+06
325	2.060E+05	2.962E+06	-5.937E+06
330	2.189E+05	2.663E+06	-6.020E+06

MicroMath Scientist 2.0 Nonlinear Least-Squares Fit

275	3.463E+05	2.951E+06	-9.717E+05
280	3.319E+05	3.737E+06	-1.783E+06
285	3.145E+05	4.277E+06	-2.815E+06
290	2.962E+05	4.470E+06	-3.852E+06
295	2.784E+05	4.380E+06	-4.705E+06
300	2.614E+05	4.146E+06	-5.307E+06
305	2.456E+05	3.872E+06	-5.687E+06
310	2.310E+05	3.613E+06	-5.905E+06
315	2.175E+05	3.387E+06	-6.013E+06
320	2.051E+05	3.194E+06	-6.052E+06
325	1.938E+05	3.029E+06	-6.046E+06
330	1.833E+05	2.888E+06	-6.013E+06



T (K)	$1/T2_{\text{red}}$ (Hz)	$\text{delta}_{\text{red}}$ (rad/s)
275	9.782E+06	3.026E+06
280	1.360E+07	-1.546E+06
285	1.653E+07	-9.867E+05
290	2.054E+07	-1.316E+06
295	2.367E+07	-6.578E+04
300	2.792E+07	-6.249E+05
305	3.092E+07	-2.960E+06
310	3.327E+07	-3.552E+06
315	3.568E+07	-2.138E+06
320	3.656E+07	-4.605E+06
325	3.553E+07	-2.697E+06
330	3.310E+07	-3.486E+06

MicroMath Scientist 2.0 Nonlinear Least-Squares Fit

275	1.068E+07
280	1.335E+07
285	1.645E+07
290	1.995E+07
295	2.372E+07
300	2.755E+07
305	3.109E+07
310	3.395E+07
315	3.573E+07
320	3.619E+07
325	3.532E+07
330	3.333E+07