Electronic Supplementary Information (ESI)

Comparative EPR Studies of Cu (II)-conjugated Phosphorous-Dendrimers in the Absence and Presence of Normal and Cancer Cells

M F. Ottaviani,[a] N. E. Brahmi,[b,c] M. Cangiotti,[a] C. Coppola,[a] F. Buccella,[a] T. Cresteil,[d] S. Mignani,[e] A. M. Caminade,[b] J. P. Costes,[b] and J. P. Majoral[b]

[a] Department of Earth, Life and Environment Sciences, Località Crocicchia, University of Urbino, 61029 Urbino, Italy

[b] CNRS, LCC (Laboratoire de Chimie de Coordination), 205 route de Narbonne, BP44099, F-31077 Toulouse Cedex 4, France

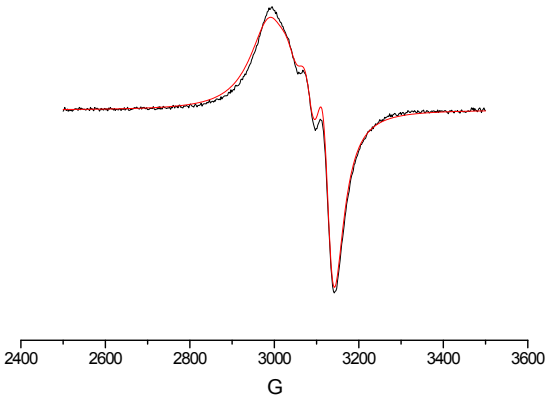
[c] Euro-Mediterranean University of Fez, Fès-Shore, Route de Sidi harazem, Fès, Morocco

[d] ICSN-CNRS UPR 2301, Avenue de la Terrasse, 91198 Gif sur Yvette, France

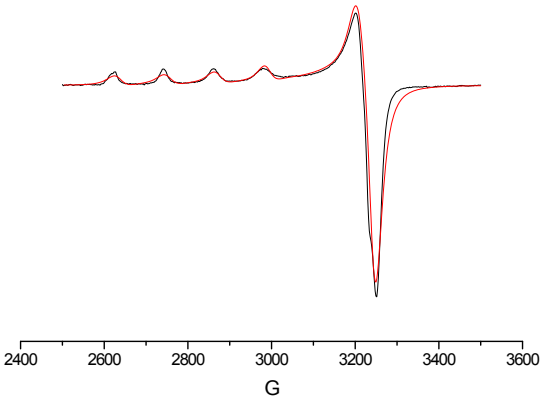
[e] Laboratoire de Chimie et de Biochimie Pharmacologiques et Toxicologique, Université Paris Descartes, PRES Sorbonne Paris Cité, CNRS UMR 860, 45, rue des Saints Pères, Paris 75006, France

Figure S1: Experimental and computed EPR spectra and components obtained after spectral subtraction for the various systems containing Cu (II) + the A, B, C ligands and dendrimers in DMF solutions, at 298 and 150 K. The main parameters obtained from computation are reported in the figures

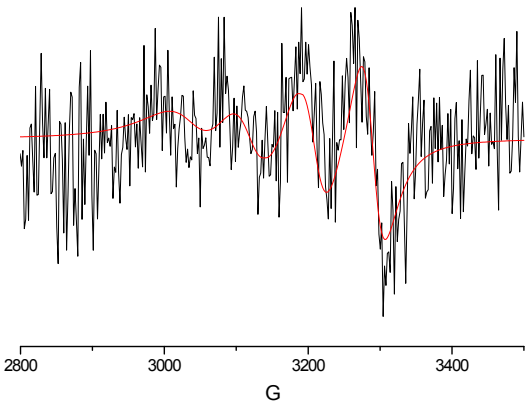
Cu-solvent 298 K
g_{ii}=2.06,2.07,2.385; A_{ii}=5,5,121 G; W_{ii}=25 G; τ=0.05 ns



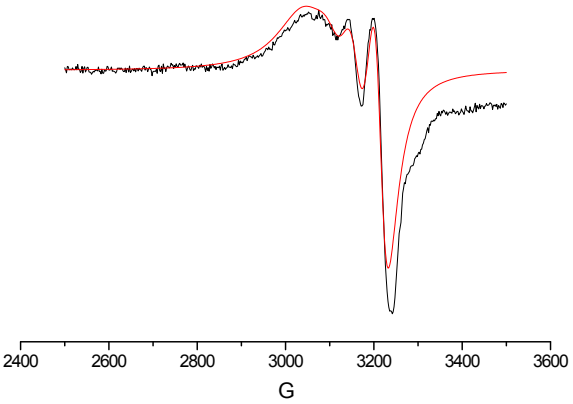
Cu-solvent 150 K
gii=2.06,2.07,2.385; Aii=5,5,121 G; Wii=15 G



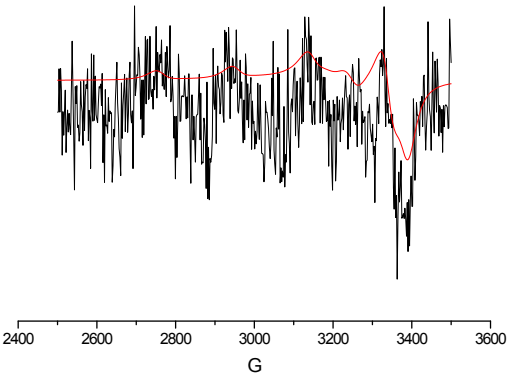
A 0.1 M + Cu 0.01 M - 298 K
g_{ii}=2.003,2.075,2.208; A_{ii}=10,50,195 G; W_{ii}=20 G; τ=0.08 ns



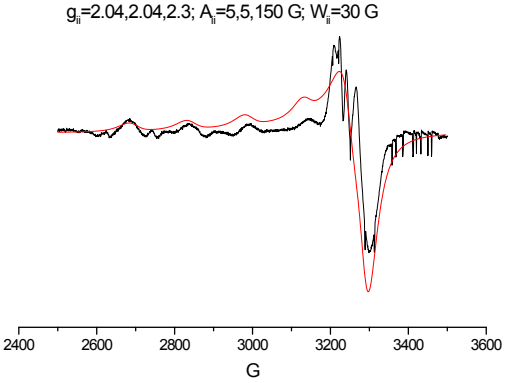
A 0.1 M + Cu 0.1 M subtracted Cu-solvent - 298 K
g_{ii}=2.04,2.04,2.3; A_{ii}=5,5,150 G; W_{ii}=25 G; τ=0.08 ns



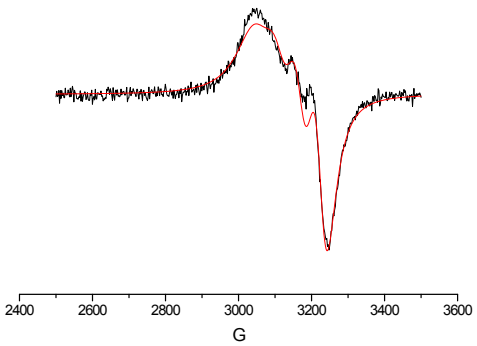
A 0.1 M + Cu 0.01 M - 150 K
g_{ii}=2.003,2.075,2.208; A_{ii}=10,50,195 G; W_{ii}=20 G



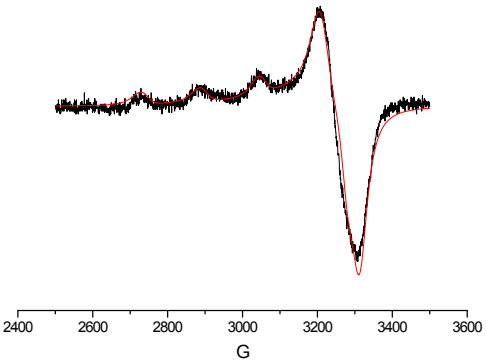
A 0.1 M + 0.1M Cu subtracted Cu-solvent - 150 K
g_{ii}=2.04,2.04,2.3; A_{ii}=5,5,150 G; W_{ii}=30 G



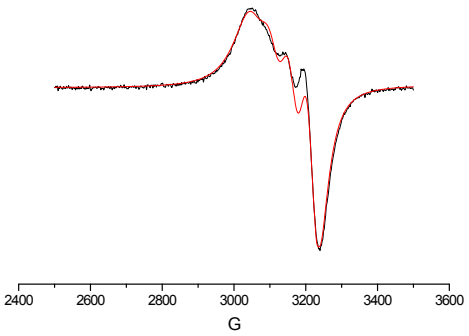
B Cu 0.03 M 298 K
g_{ii}=2.03,2.064,2.256; A_{ii}=5,5,160 G; W_{ii}=25 G; τ=0.07 ns; Wex=3.2x10^{8} s^{-1}



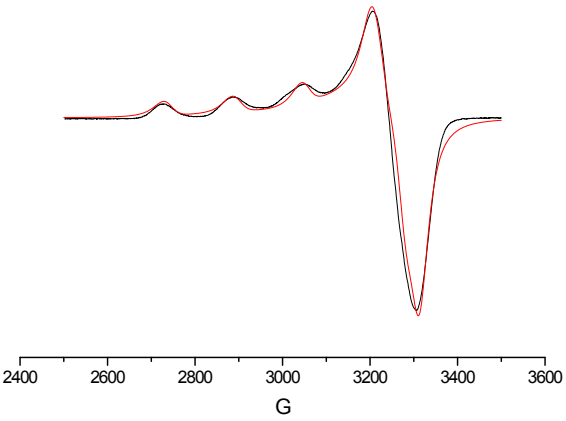
B Cu 0.03 M 150 K
g_{ii}=2.03,2.064,2.256; A_{ii}=5,5,160 G; W_{ii}=20 G



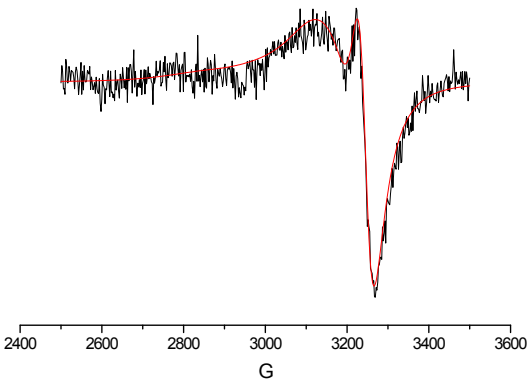
B Cu 0.1 M 298 K
g_{ii}=2.031,2.065,2.26; A_{ii}=5,5,153 G; W_{ii}=25 G; τ=0.07 ns; Wex=3.2x10^{8} s^{-1}



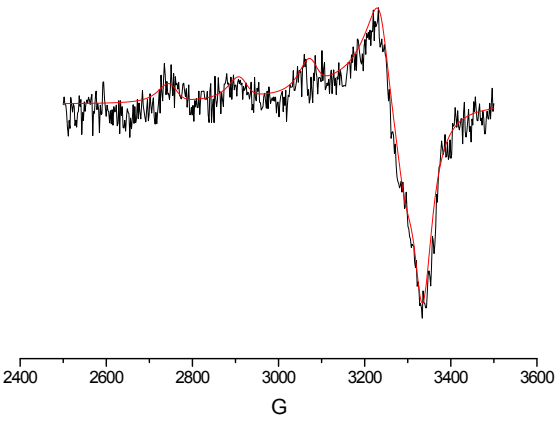
B Cu 0.1 M 150 K
g_{ii}=2.031,2.065,2.26; A_{ii}=5,5,153 G; W_{ii}=25 G



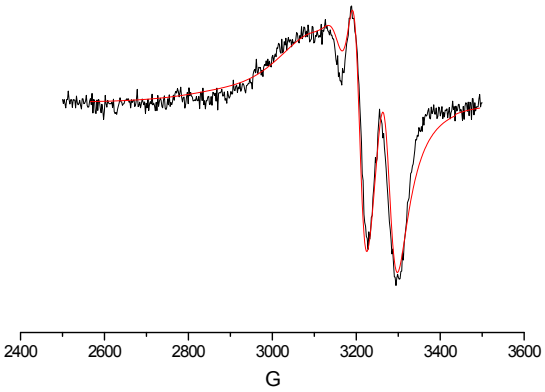
C 0.1 M + Cu up to 0.05M 298 K
g_{ii}=2.016,2.052,2.233; A_{ii}=10,10,165 G; W_{ii}=28 G
τ = 0.3 ns



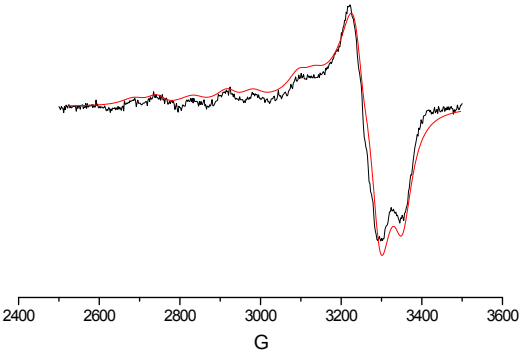
C 0.1 M + Cu 0.05M 150 K
g_{ii}=2.0156,2.052,2.233; A_{ii}=10,10,165 G; W_{ii}=20 G



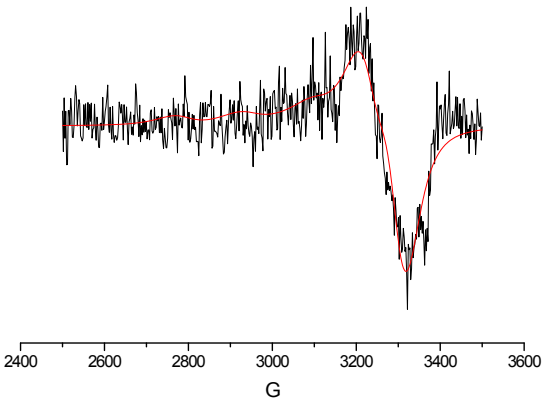
C 0.1 M + 0.1M Cu - 298 K
50%: gii=2.006,2.048,2.221; Aii=5,5,178G; Wii=25 G; τ=0.4 ns
50%: gii=2.04,2.04,2.3; Aii=5,5,150 G; Wii=30 G; τ=0.12 ns



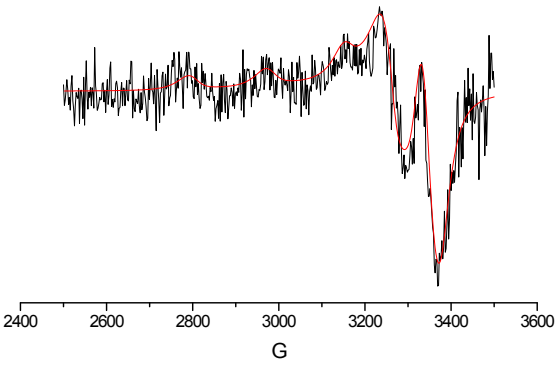
C 0.1 M + 0.1M Cu 150 K
50%: gii=2.006,2.048,2.221; Aii=5,5,178G; Wii=20 G
50%: gii=2.04,2.04,2.3; Aii=5,5,150 G; Wii=30 G



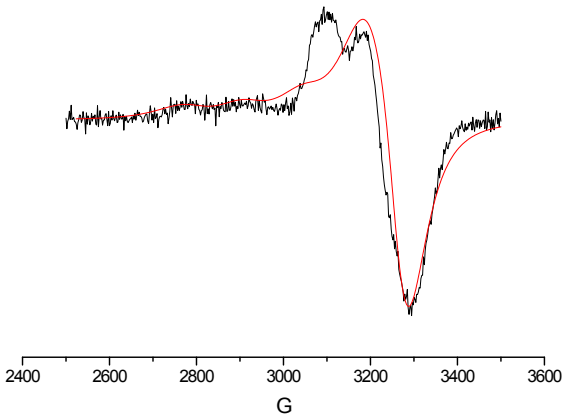
G2A 0.1 M + Cu 0.01 M subtracted Cu-solvent - 298 K
g_{ii}=2.008,2.05,2.22; A_{ii}=5,5,170 G; W_{ii}=25 G; τ= 3.3 ns



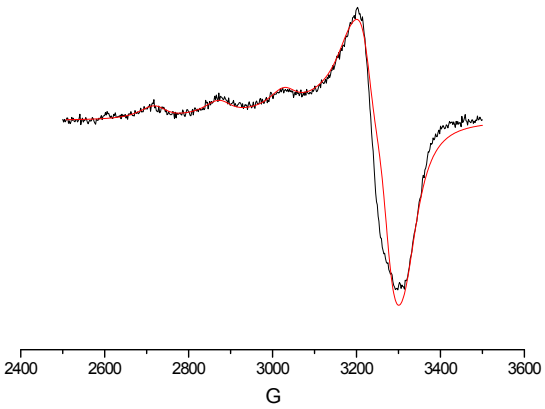
G2A Cu 0.05 M 150 K (at 298 K, 8 ns)
g_{ii}=2.03,2.04,2.18; A_{ii}=5,5,182 G; W_{ii}=25 G



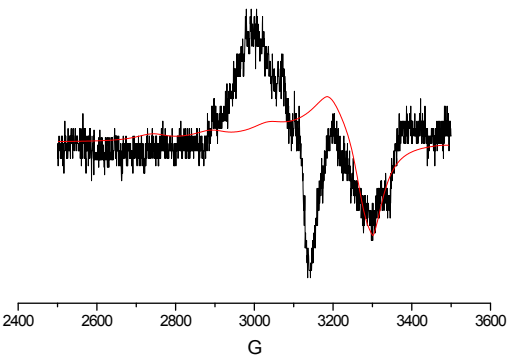
G2A Cu 0.05 M 150 K
50 %: g_{ii}=2.035,2.073,2.28; A_{ii}=5,5,156 G; W_{ii}=35 G; τ = 1.05 ns



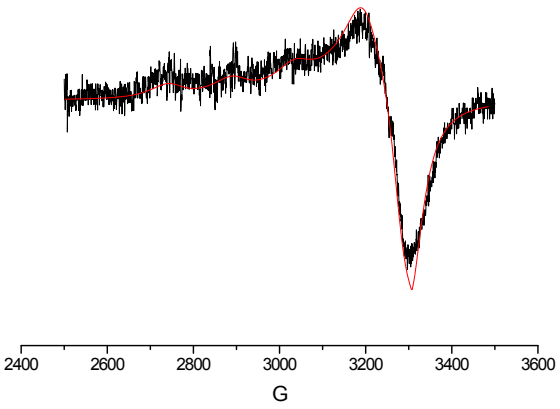
G2A Cu 0.05 M 150 K
50 %: g_{ii}=2.035,2.073,2.28; A_{ii}=5,5,156 G; W_{ii}=35 G



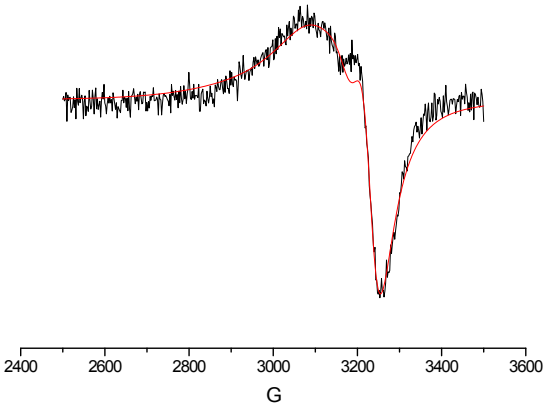
G3A 0.1 M + 0.1M Cu - 298 K
g_{ii}=2.032,2.07,2.272; A_{ii}=5,5,145 G; Wii=35 G; τ=4 ns



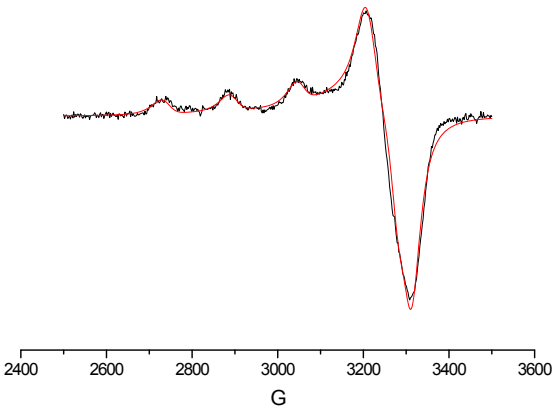
G3A 0.1 M + 0.1M Cu subtracted Cu-solvent - 150 K
g_{ii}=2.032,2.07,2.272; A_{ii}=5,5,145 G; Wii=35 G



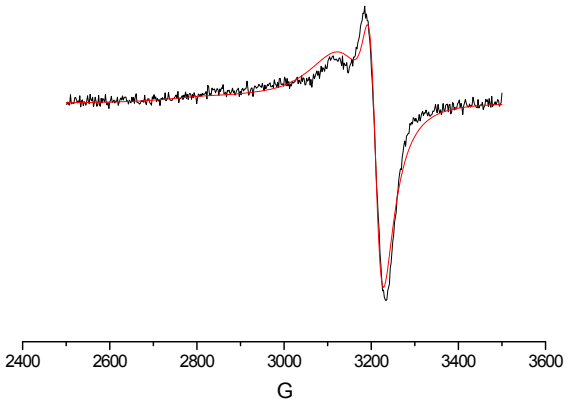
G1B Cu 0.05 M 298 K (similar spectrum at lower concentrations)
g_{ii}=2.03,2.064,2.256; A_{ii}=5,5,160 G; W_{ii}=40 G; τ=0.2 ns



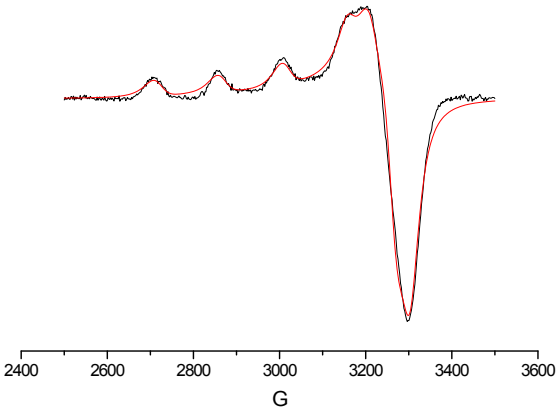
G1B Cu 0.05 M 150 K (similar spectrum at lower concentrations)
g_{ii}=2.03,2.064,2.256; A_{ii}=5,5,160 G; W_{ii}=20 G



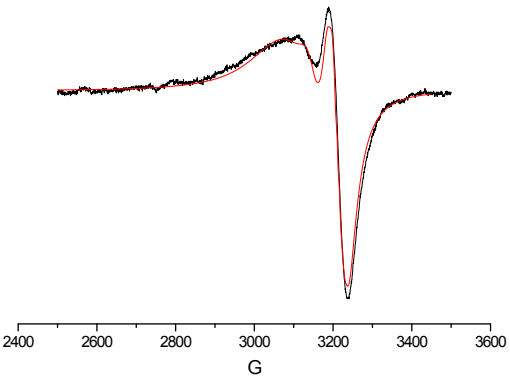
G1B Cu 0.1 M 298 K
60%: g_{ii}=2.038,2.076,2.29; A_{ii}=5,5,151 G; W_{ii}=17 G; τ=0.35 ns



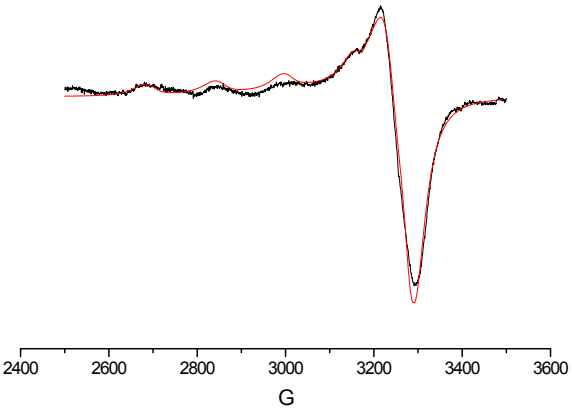
G1B Cu 0.1 M 150 K
60%: g_{ii}=2.038,2.076,2.29; A_{ii}=5,5,151 G; W_{ii}=20 G



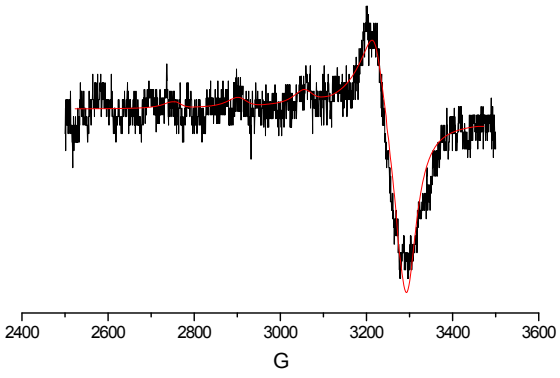
G2B 0.1 M - Cu 0.05M - 298 K
g_{ii}=2.04,2.05,2.288; A_{ii}=5,5,163 G; W_{ii}=25 G; τ=0.33 ns



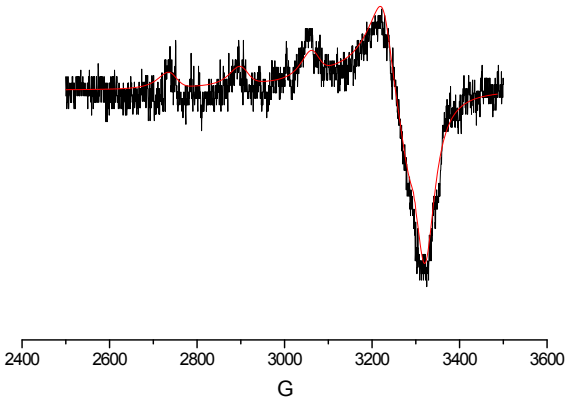
G2B 0.1 M - Cu 0.05M - 150 K
g_{ii}=2.04,2.05,2.288; A_{ii}=5,5,163 G; W_{ii}=25 G

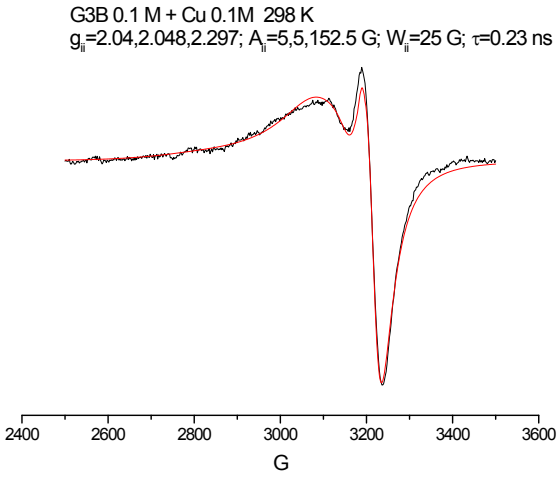


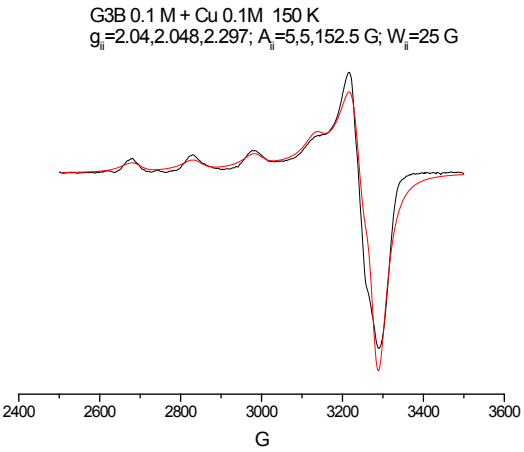
G3B 0.1 M - Cu 0.03M - 298 K
g_{ii}=2.021,2.06,2.255; A_{ii}=5,5,160 G; W_{ii}=20 G; τ=7 ns

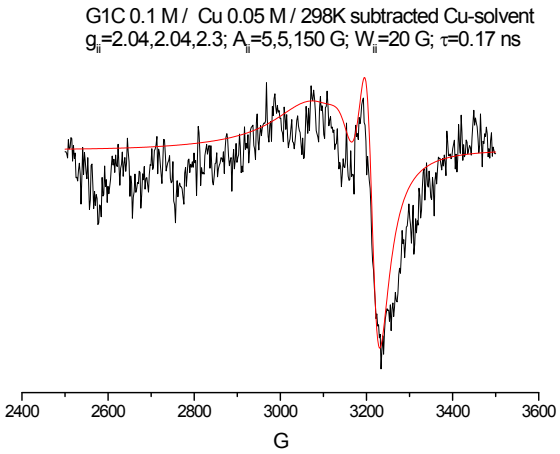


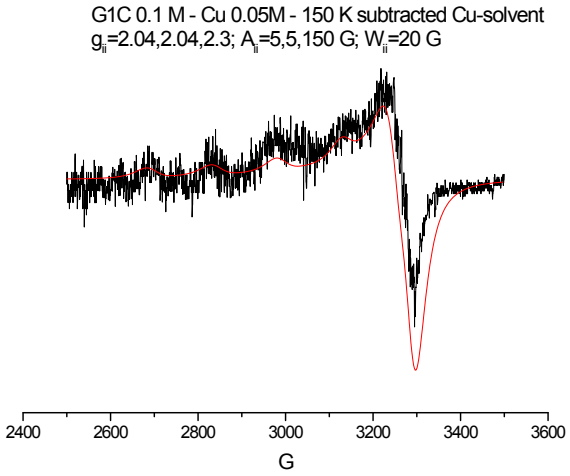
G3B 0.1 M - Cu 0.03M - 150 K
g_{ii}=2.021,2.06,2.255; A_{ii}=5,5,160 G; W_{ii}=20 G




G3B 0.1 M + Cu 0.1M 298 K
g_{ii}=2.04,2.048,2.297; A_{ii}=5,5,152.5 G; W_{ii}=25 G; τ=0.23 ns
2400
2600
2800
3000
3200
3400
3600
G


G3B 0.1 M + Cu 0.1M 150 K
g_{ii}=2.04,2.048,2.297; A_{ii}=5,5,152.5 G; W_{ii}=25 G
2400
2600
2800
3000
3200
3400
3600
G


G1C 0.1 M / Cu 0.05 M / 298K subtracted Cu-solvent
g_{ii}=2.04,2.04,2.3; A_{ii}=5,5,150 G; W_{ii}=20 G; τ=0.17 ns
2400
2600
2800
3000
3200
3400
3600
G


G1C 0.1 M - Cu 0.05M - 150 K subtracted Cu-solvent
g_{ii}=2.04,2.04,2.3; A_{ii}=5,5,150 G; W_{ii}=20 G
2400
2600
2800
3000
3200
3400
3600
G

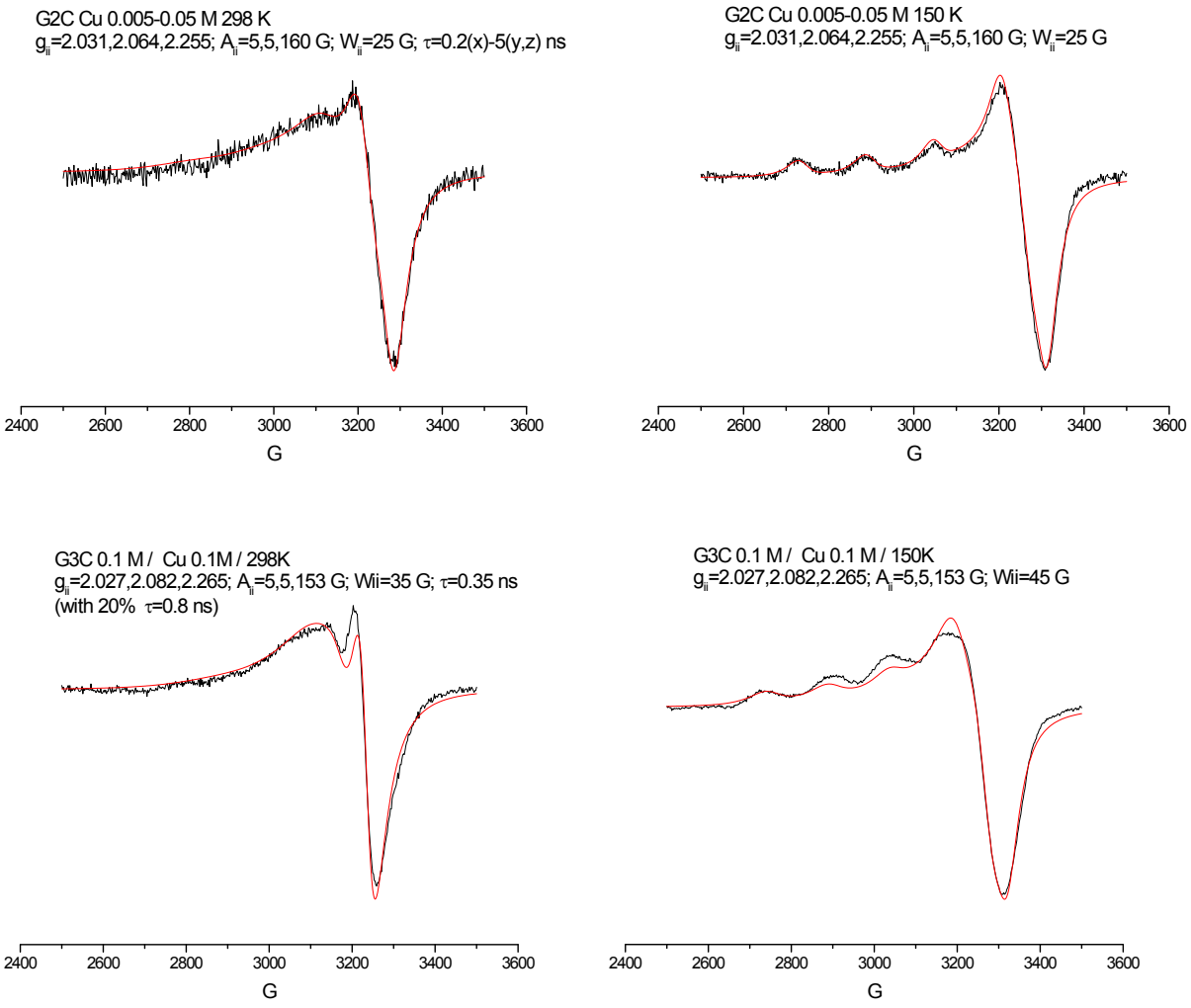
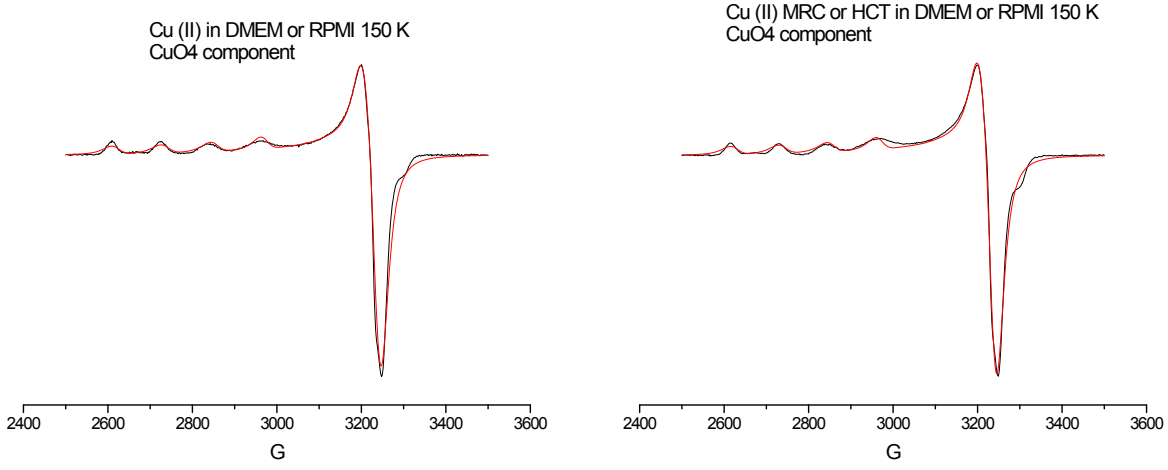
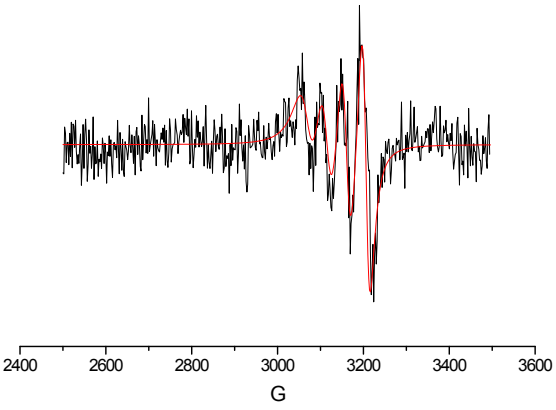


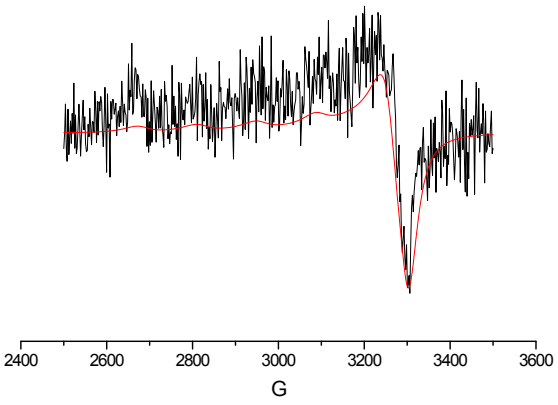
Figure S2: Experimental and computed EPR spectra and components obtained after spectral subtraction at 298 and 150 K for the various systems containing Cu (II) at 0.05 M concentration added to **G3B** dendrimer at concentration of 0.1 M and MRC or HCT cells in DMEM or RPMI media, respectively. Both binary and ternary mixtures were analyzed. The main parameters are reported in Table 2



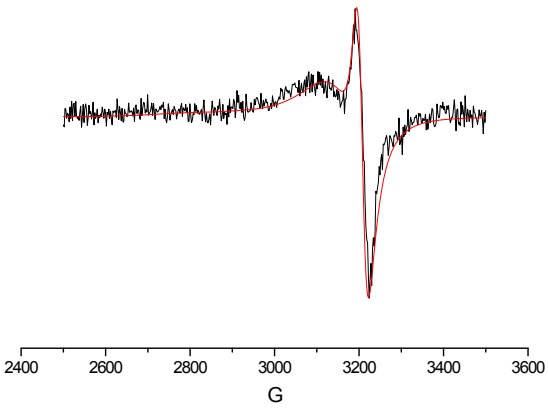
Cu (II) in DMEM or RPMI 298 K - Subtracted CuO4



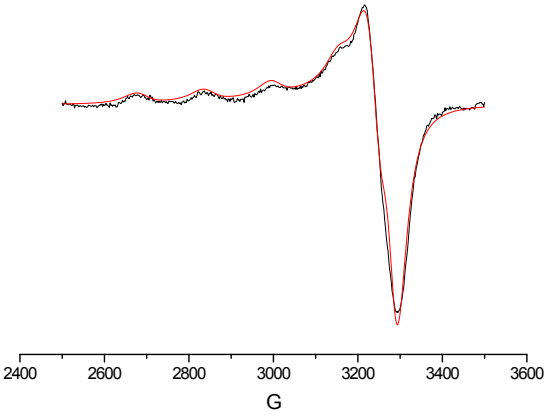
Cu (II) in DMEM or RPMI 150 K - Subtracted CuO4



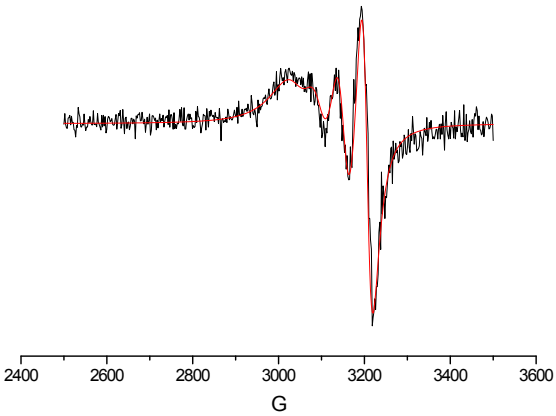
Cu (II) - G3B in DMEM or RPMI 298 K - Subtracted CuO4



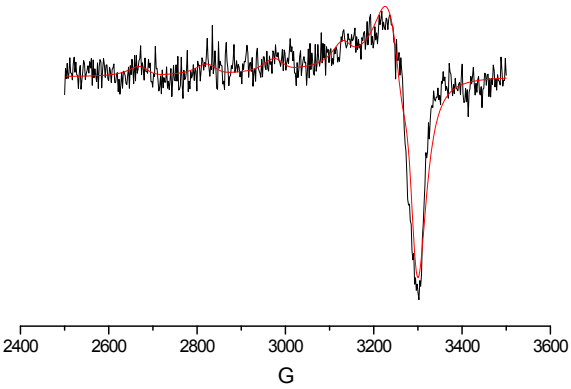
Cu (II) - G3B in DMEM or RPMI 150 K - Subtracted CuO4

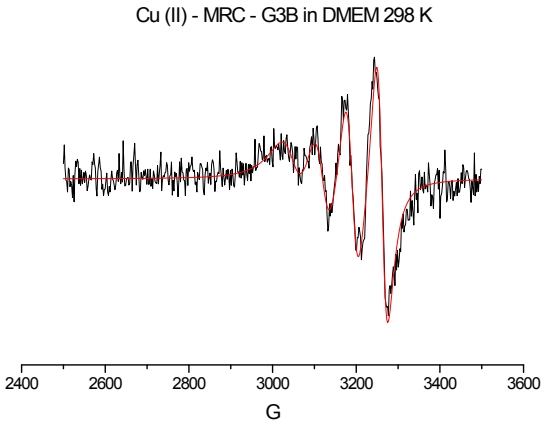


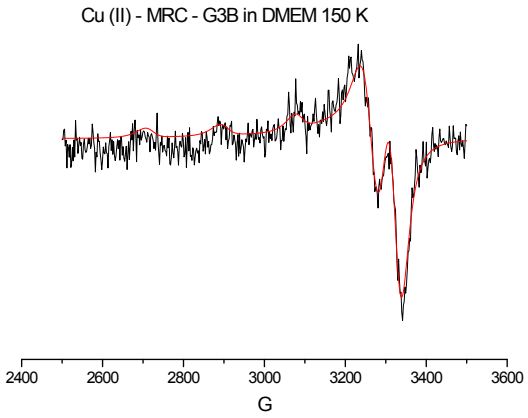
Cu (II) - MRC in DMEM 298 K - Subtracted CuO4
Equivalent subtracted signal for HCT in RPMI

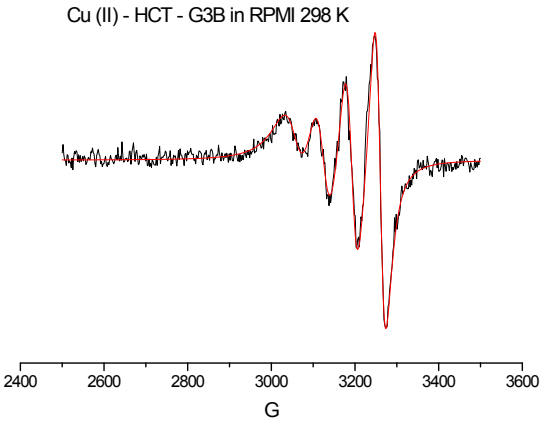


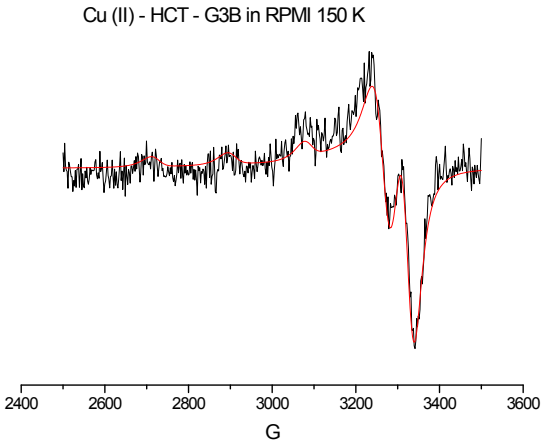
Cu (II) - MRC in DMEM 150 K - Subtracted CuO4
Equivalent subtracted signal for HCT in RPMI




Cu (II) - MRC - G3B in DMEM 298 K
2400
2600
2800
3000
3200
3400
3600
G


Cu (II) - MRC - G3B in DMEM 150 K
2400
2600
2800
3000
3200
3400
3600
G


Cu (II) - HCT - G3B in RPMI 298 K
2400
2600
2800
3000
3200
3400
3600
G


Cu (II) - HCT - G3B in RPMI 150 K
2400
2600
2800
3000
3200
3400
3600
G