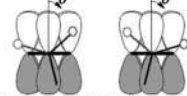




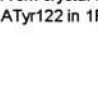
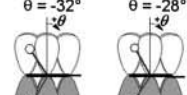



Correction

Svistunenko, Dimitri A., and Chris E. Cooper. 2004. A new method of identifying the site of tyrosyl radicals in proteins. *Biophys. J.* 87:582–595.

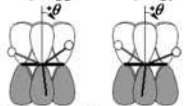

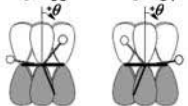

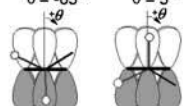
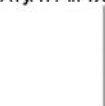
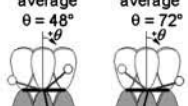

Table 1 did not print correctly. The correct table is as follows:

TABLE 1 The simulation of the HF and X-band EPR spectra of tyrosyl radical in different proteins

1. <i>Salmonella typhimurium</i> Ribonucleotide Reductase 244.997 GHz spectrum, $A_m = 15$ G (Allard et al., 1996)			9.454 GHz spectrum, $A_m = 2.6$ G (Allard et al., 1996)			From simulation: $\theta = 47^\circ$ $\theta = 73^\circ$  From crystal structure: ATyr105 in 1R2F; $\theta = 41.5^\circ$ 
The algorithm input parameters: $p_{C1} = 0.350 \pm 0.002$ $\theta = 47^\circ(\text{or } 73^\circ) \pm 4^\circ$						
2. <i>Paracoccus Denitrificans</i> Cytochrome c Oxidase + H_2O_2 The experimental HF spectrum is not known; the simulation is for 285 GHz; $A_m = 3$ G			X-band spectrum, $A_m = 2$ G (MacMillan et al., 1999)			From simulation: $\theta = -38^\circ$ $\theta = -22^\circ$  From crystal structure: ATyr167 in 1QLE; $\theta = -39.5^\circ$ 
The algorithm input parameters: $p_{C1} = 0.355 \pm 0.009$ $\theta = -38^\circ(\text{or } -22^\circ) \pm 2^\circ$						
3. <i>Escherichia coli</i> Ribonucleotide Reductase 285 GHz spectrum (Dorlet et al., 2002)			X-band spectrum (Hoganson & Babcock, 1992)			From simulation: $\theta = -69^\circ$ $\theta = 9^\circ$  From crystal structure: ATyr122 in 1RIB; $\theta = 7.7^\circ$ 
The algorithm input parameters: $p_{C1} = 0.358 \pm 0.002$ $\theta = -69^\circ(\text{or } 9^\circ) \pm 2^\circ$						
4. Horse heart metMb + H_2O_2 The experimental HF spectrum is not known; the simulation is for 285 GHz; $A_m = 3$ G			9.510 GHz spectrum, $A_m = 2$ G (Miki et al., 1989)			From simulation: $\theta = -32^\circ$ $\theta = -28^\circ$  From crystal structure: Tyr103 in 1WLA; $\theta = -31.7^\circ$ 
The algorithm input parameters: $p_{C1} = 0.370 \pm 0.010$ $\theta = -32^\circ(\text{or } -28^\circ) \pm 2^\circ$						

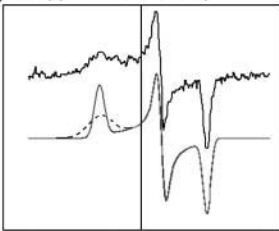
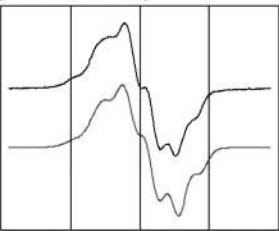
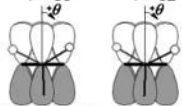

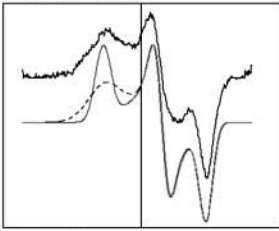
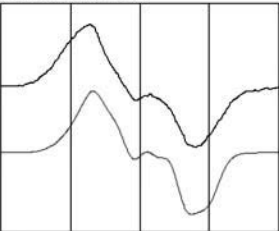
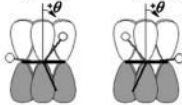

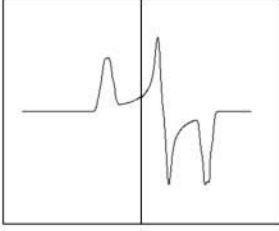
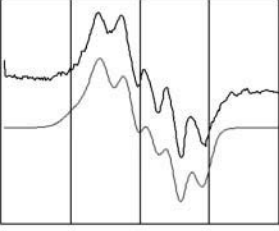
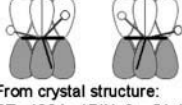

(Continued)

TABLE 1 (Continued)

5. Human metHb + H₂O₂ The experimental HF spectrum is not known; the simulation is for 285 GHz; $A_m = 3$ G	9.797465 GHz spectrum, $A_m = 2$ G (Svistunenko et al., 2002)	From simulation: $\theta = 53^\circ$ $\theta = 67^\circ$  From crystal structure: CTyr42 in 1HGB; $\theta = 49.8^\circ$ 
The algorithm input parameters: $p_{C1} = 0.375 \pm 0.010$ $\theta = 53^\circ(\text{or } 67^\circ) \pm 2^\circ$		
6. Ovine prostaglandin H synthase, "narrow singlet" (indomethacin-inhibited) 285 GHz spectrum, $A_m = 20$ G (Dorlet et al., 2002)	9 GHz spectrum, $A_m = 3$ G (Dorlet et al., 2002)	From simulation: $\theta = 39^\circ$ $\theta = 81^\circ$  From crystal structure: ATyr495 in 1PGF; $\theta = 38.0^\circ$ 
--- $\Delta H_k \times 2.2$ The algorithm input parameters: $p_{C1} = 0.380 \pm 0.003$ $\theta = 39^\circ(\text{or } 81^\circ) \pm 2^\circ$		
7. Mouse TA3 tumour cells, overproducing M2 subunit of mammalian RNR 244.997 GHz spectrum, $A_m = 3$ G (Schmidt et al., 1996)	9.5 GHz spectrum (Sahlin et al., 1987)	From simulation: $\theta = -63^\circ$ $\theta = 3^\circ$  From crystal structure: ATyr177 in 1XSM; $\theta = 18.3^\circ$ 
The algorithm input parameters: $p_{C1} = 0.388 \pm 0.002$ $\theta = -63^\circ(\text{or } 3^\circ) \pm 2^\circ$		
8. Photosystem II Y_D[•] radical 285.363 GHz spectrum, $A_m = 3.3$ G; <i>S. oleracea</i> (Dorlet et al., 2000)	9.472911 GHz spectrum, $A_m = 1$ G <i>A. thaliana</i> (Svistunenko et al., 2002)	From simulation: average $\theta = 48^\circ$ average $\theta = 72^\circ$  The crystal structure is not known 
The algorithm input parameters: $p_{C1} = 0.395 \pm 0.002$ (both spectra); $\theta = 47^\circ(\text{or } 73^\circ) \pm 3^\circ$ for <i>S. oleracea</i> (HF spectrum) and $\theta = 49^\circ(\text{or } 71^\circ) \pm 3^\circ$ for <i>A. thaliana</i> (X-band spectrum); Angle between β -protons 117° in both cases#		

(Continued)

TABLE 1 (Continued)

9. Bovine liver catalase + peroxyacetic acid 284.35 GHz spectrum, $A_m = 10$ G; pH 5.2; (Ivancich et al., 1999)		
		From simulation: $\theta = 58^\circ$ $\theta = 62^\circ$  From crystal structure: CTyr369 in 4BLC; $\theta = 58.4^\circ$ 
--- $\Delta H_x \times 4$ The algorithm input parameters: $\rho_{C1} = 0.411 \pm 0.004$ $\theta = 58^\circ(\text{or } 62^\circ) \pm 3^\circ$		
10. Ovine prostaglandin H synthase, "wide doublet" (active cyclooxygenase) 285 GHz spectrum, $A_m = 20$ G (Dorlet et al., 2002)		
		From simulation: $\theta = 37^\circ$ $\theta = 83^\circ$  From crystal structure: ATyr385 in 1EQG; $\theta = 26.9^\circ$ 
--- $\Delta H_x \times 2.7$ The algorithm input parameters: $\rho_{C1} = 0.416 \pm 0.003$ $\theta = 37^\circ(\text{or } 83^\circ) \pm 3^\circ$		
11. Soybean metLb + H_2O_2 The experimental HF spectrum is not known; the simulation is for 285 GHz; $A_m = 3$ G		
		From simulation: $\theta = 45^\circ$ $\theta = 75^\circ$  From crystal structure: BTyr133 in 1BIN; $\theta = 51.4^\circ$ 
The algorithm input parameters: $\rho_{C1} = 0.420 \pm 0.015$ $\theta = 45^\circ(\text{or } 75^\circ) \pm 3^\circ$		

In each box, the simulated spectrum is shown below the experimental one. All experimental spectra are taken from the literature. When experimental spectrum is not available, only the simulated one is present. In three cases (6, 9, and 10), the dashed trace corresponds to the spectrum simulated for a greater than the algorithm predicts x -component of the linewidth, all other parameters being generated by the algorithm. The optimal values of the algorithm input parameters ρ_{C1} and θ , used to calculate the simulation parameters (see Supplementary Material, *Simulation Data*), are indicated under the spectra. The radicals in the table are arranged by ascending ρ_{C1} . For each radical, the two optimal θ -angles, equivalent in terms of providing the simulation parameters, are compared with the θ -angle found from the crystal structure, the latter shown under the corresponding optimal angle. The tyrosine number and the Protein Data Bank (<http://www.rcsb.org/pdb/>) file, e.g., 1R2F for *S. typhimurium* RNR (Eriksson et al., 1998), are indicated. Other structure files quoted in the table were first presented in the articles: 1QLE (Harrenga and Michel, 1999), 1RIB (Nordlund and Eklund, 1993), 1WLA (Maurus et al., 1997), 1HGB (Liddington et al., 1992), 1PGF (Loll et al., 1996), 1XSM (Kauppi et al., 1996), 4BLC (Ko et al., 1999), 1EQG (Selinsky et al., 2001), and 1BIN (Hargrove et al., 1997). The details of 1), how the errors in optimal ρ_{C1} and θ were determined; 2), how the spectra were plotted on a common magnetic field axis; and 3), how the θ -values were found from the crystal structure, are all described in Software and Methods.

[#]The algorithm (available in Supplementary Material as the file calculator *algorithm.xls*) allows us to vary the angle between the projections of the bonds $C_\beta-H_{\beta1}$ and $C_\beta-H_{\beta2}$ to the $y-z$ plane (default value is 120°). The photosynthetic Y_D radical is the only occasion when we exercised this option.