CONFORMATIONAL ANALYSIS OF QUININE AND ITS PSEUDO ENANTIOMER QUINIDINE: A COMBINED JET-COOLED SPECTROSCOPY AND VIBRATIONAL CIRCULAR DICHROISM STUDY.

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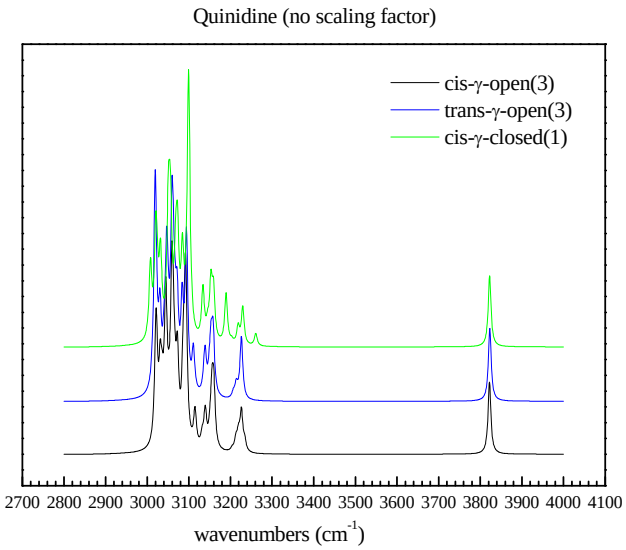

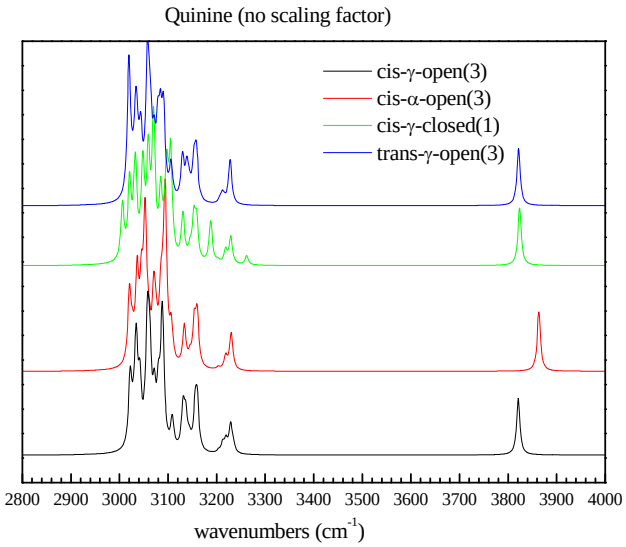

Figure S1: Spectra of the most stable conformers of quinine and quinidine in the gas phase calculated at the b3lyp/6-31G+(d,p) level of theory. No scaling factor has been applied

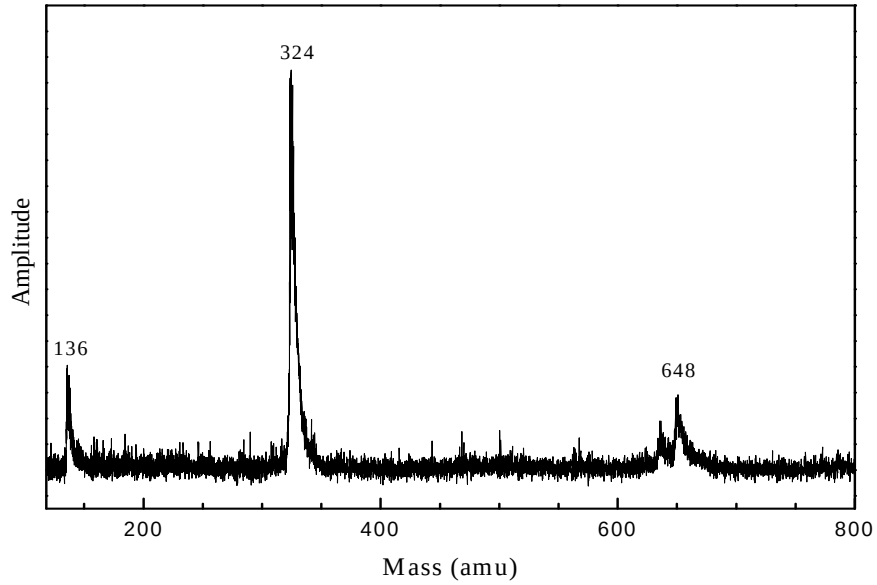

Figure S2: Time of Flight Mass Spectrum showing the monomer, dimer, and fragment of quinine.(λ_{exc}= 318 nm and λ_{ion}=266 nm)

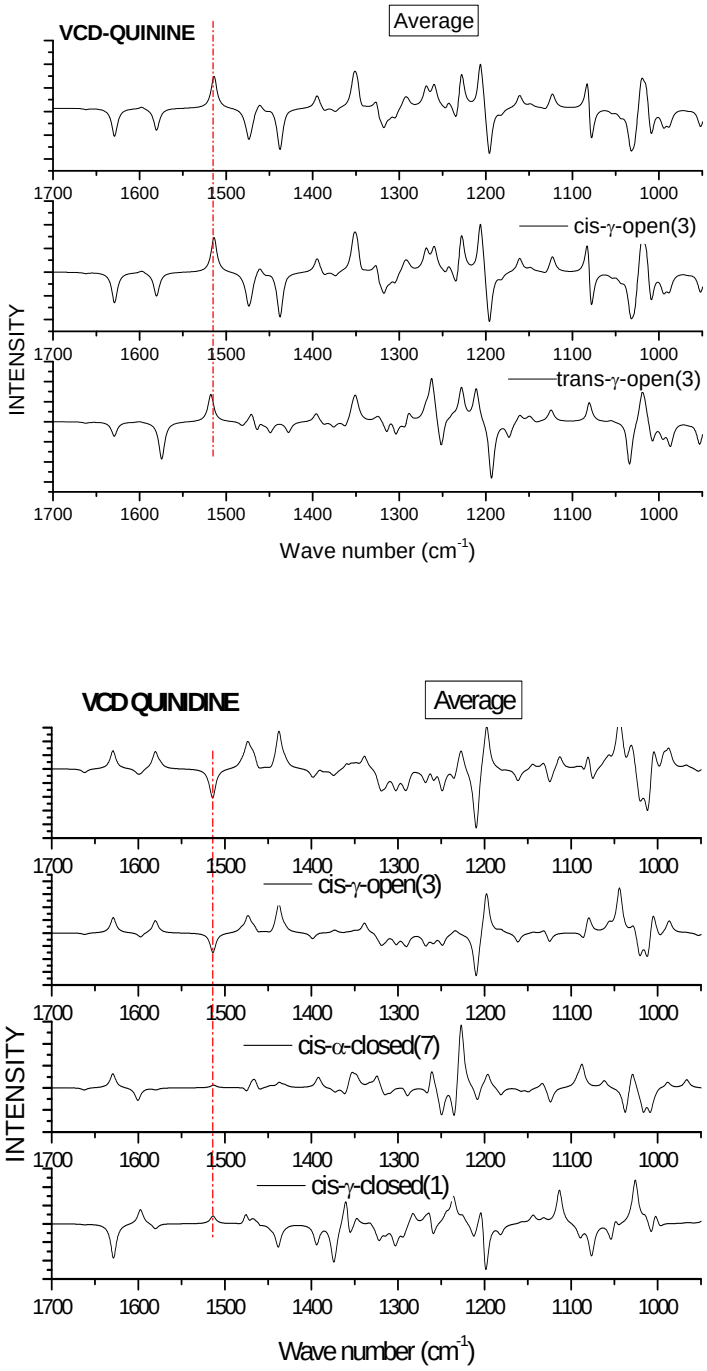

Figure S3: Illustrative VCD spectra of different conformers of quinine (top) and quinidine (bottom) calculated at the b3lyp/6-31G+(d,p) level of theory. A scaling factor of 0.98 has been applied. Please note that all the conformers of quinine being of the γ-open type display the same VCD spectrum below 1500 cm^{-1}, while some conformers of quinidine being of α or closed type may exhibit an inversion in sign of the bands relative to the main conformer. The same holds around 1200 cm^{-1}.

Reference (24) is:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X. J.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A. ; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. S. *GAUSSIAN 09, REVISION A.02*; Gaussian Inc.: Wallingford CT, **2009**.