

The Value of Universally Available Raw NMR Data for Transparency, Reproducibility, and Integrity in Natural Product Research

James B. McAlpine,^{a*} Shao-Nong Chen,^a Andrei Kutateladze,^b John B. MacMillan,^c Giovanni Appendino,^d Andersson Barison,^e Mehdi A. Beniddir,^f Maique W. Biavatti,^g Stefan Bluml,^h Asmaa Boufridi,ⁱ Mark S. Butler,^j Robert J. Capon,^j Young H. Choi,^k David Coppage,^c Phillip Crews,^c Michael T. Crimmins,^l Marie Csete,^m Pradeep Dewapriya,^j Joseph M. Egan,ⁿ Mary J. Garson,^o Grégory Genta-Jouve,^p William H. Gerwick,^{q,r} Harald Gross,^s Mary Kay Harper,^t Precilia Hermanto,^u James M. Hook,^u Luke Hunter,^u Damien Jeannerat,^v Nai-Yun Ji,^w Tyler A. Johnson,^c David G. I. Kingston,^x Hiroyuki Koshino,^y Hsiau-Wei Lee,^c Guy Lewin,^f Jie Li,^f Roger G. Linington,ⁿ Miaomiao Liu,ⁱ Kerry L. McPhail,^z Tadeusz F. Molinski,^{aa} Bradley S. Moore,^{q,r} Joo-Won Nam,^{ab} Ram P. Neupane,^{ac} Matthias Niemitz,^{ad} Jean-Marc Nuzillard,^{ae} Nicholas H. Oberlies,^{af} Fernanda M. M. Ocampos,^e Guohui Pan,^{ag} Ronald J. Quinn,ⁱ D. Sai Reddy,^b Jean-Hugues Renault,^{ae} José Rivera-Chávez,^{ah} Wolfgang Robien,^{ai} Carla M. Saunders,^{aj} Thomas J. Schmidt,^{ak} Christoph Seger,^{al} Ben Shen,^{ag} Christoph Steinbeck,^{am} Hermann Stuppner,^{al} Sonja Sturm,^{al} Orazio Tagliatalata-Scafati,^{an} Dean J. Tantillo,^{aj} Robert Verpoorte,^k Bin-Gui Wang,^{ar} Craig M. Williams,^o Philip G. Williams,^{ac} Julien Wist,^{ao} Jian-Min Yue,^{ap} Chen Zhang,^{aq} Zhengren Xu,^{ag} Charlotte Simmler,^a David C. Lankin,^a Jonathan Bisson,^a Guido F. Pauli^{a*}

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SI1. Spectroscopic Data of the Fluorinated Amino Acids

^1H (600 MHz, CDCl_3): Major isomer (~55%): 4.589 (dd, $J = 9.2$ and 5.2 Hz); 3.844 (dd, $J = 13.1$ and 12.2 Hz); 3.778 (dd, $J = 13.1$ and 12.2 Hz); 2.716 (ddd, $J = 14.3, 13.1$ and 9.2 Hz); 2.659 (ddd, $J = 14.3, 13.1$ and 5.2 Hz); 1.500 (s); Minor isomer (~45%): 4.494 (dd, $J = 9.2$ and 5.2 Hz); 3.896 (dd, $J = 13.1$ and 12.2 Hz); 3.829 (dd, $J = 13.1$ and 12.2 Hz); 2.778 (ddd, $J = 13.7, 13.1$ and 9.2 Hz); 2.659 (ddd or dq, $J = 13.7, 13.1$ and 5.2 Hz); 1.450 (s)

^1H -decoupled ^{19}F (600 MHz [^1H], CDCl_3): Major isomer: -99.470 (s, $w_{1/2} \sim 17.7$ Hz); minor isomer: -99.632 (s, $w_{1/2} \sim 9.5$ Hz)

^{19}F (600 MHz [^1H], CDCl_3): Major isomer: -99.470 (p, $^3J_{\text{H-F}} \sim 13.1$ Hz); minor isomer: -99.632 (p, $^3J_{\text{H-F}} \sim 13.1$ Hz)