An Advanced NMR-based Structural Investigation of Glucosinolates and Desulfoglucosinolates

Nada Ibrahim,[†] Ingrid Allart-Simon,[†] Gina R. De Nicola,[‡] Renato Iori,[‡] Jean-Hugues Renault,[†] Patrick Rollin,[§] and Jean-Marc Nuzillard.[*,†]

† Université de Reims Champagne-Ardenne and CNRS, Institut de Chimie Moléculaire de Reims, UMR 7312, SFR CAP'SANTE, F-51687 Reims, France.

‡ Consiglio per la Ricerca in Agricoltura e l'Analisi dell'Economia Agraria, Agricoltura e Ambiente (CREA-AA), Via di Corticella 133, 40128 Bologna, Italy

§ Université d'Orléans and CNRS, Institut de Chimie Organique et Analytique, UMR 7311, BP 6759, F-45067 Orléans, France.

Data files mentioned below are stored at http://doi.org/10.5281/zenodo.1069439

Data_1H_13C_15N.zip: this archive contains acquisition and processed files in Bruker format from which 1D NMR data of the studied compounds have been obtained. Datasets are named after compound codes, as defined in Table 1 of article text. Acquisition folder (acqu) "1" is for ^{1}H NMR with processing folder "1" for original spectra and "999" for spectra reconstruction by PERCH after NMR parameter extraction. Acqu "2" is for ^{13}C NMR spectra. Acqu "301" is like "1" but was recorded immediately before the ^{1}H-^{15}N spectra were recorded. Acqu "302" and "303" respectively contain the high- and low-resolution ^{1}H-^{15}N HMBC spectra.

Data_2D_NMR.zip: this archive contains ^{1}H (acqu "1"), ^{13}C (acqu "2"), ^{1}H-^{1}H COSY (acqu "3"), ^{1}H-^{13}C HSQC (acqu "4") and ^{1}H-^{13}C HMBC (acqu "5") spectra from which ^{1}H and ^{13}C NMR chemical shifts were assigned.

SDF.zip: this archive file contains the SDF files of the studied molecules.

GLs.txt: Text file (not a text processor file) that contains the NMR parameters of all the studied molecules.

GLs.xlsx: Excel file that contains the NMR parameters of all the studied molecules.

GLs.db: Molecular structures and NMR parameters of the studied compounds stored in a SQLite database file.

SupportingInformation.pdf: this file.