

Supporting Information:

Experimental and Theoretical Evaluation of *trans*-3-Halo-2-Hydroxy-Tetrahydropyran Conformational Preferences. Beyond Anomeric Interaction.

Thaís M. Barbosa^a, Renan, V. Viesser^a, Raymond J. Abraham^b, Roberto Rittner^{a*} and

Cláudio F. Tormena^a

^a*Chemistry Institute, University of Campinas - UNICAMP – P. O. Box: 6154, 13083-970 - Campinas - SP – Brazil. e-mail: rittner@iqm.unicamp.br*

^b*Department of Chemistry, University of Liverpool – P. O. Box: 147, L69 3BX – Liverpool - UK*

Fluorohydrin (*cis* and *trans*)

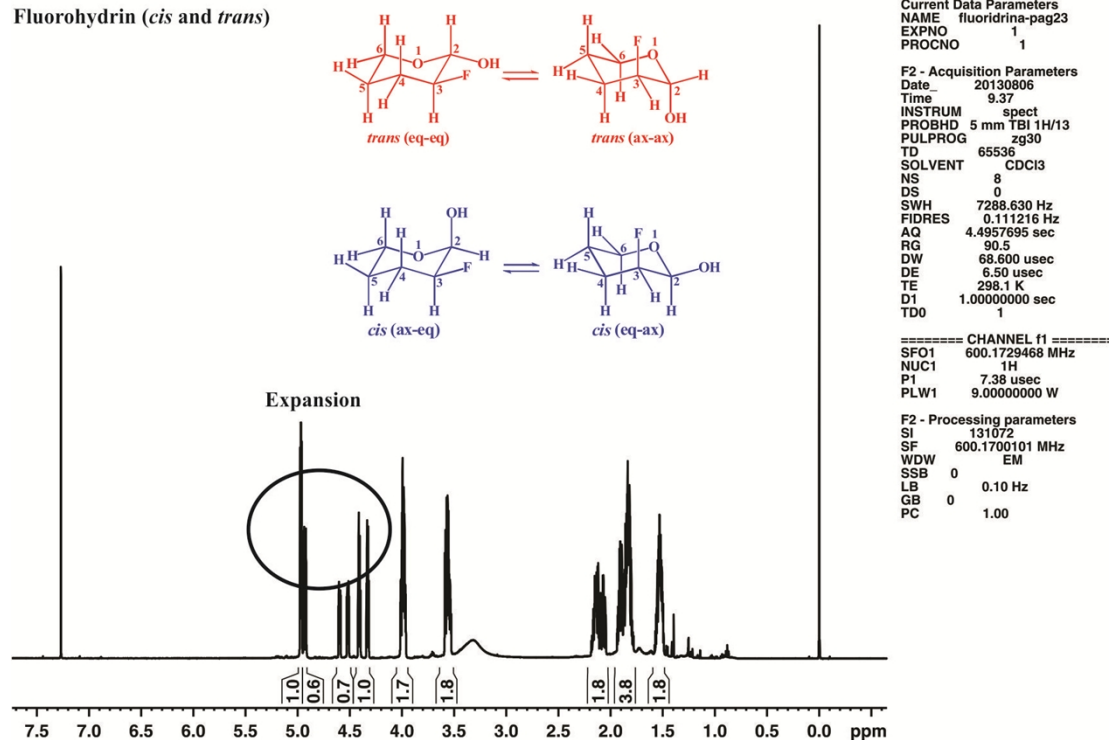


Figure S1: ^1H NMR spectrum of the mixture (*cis* and *trans*) fluorohydrin in CDCl_3 acquired at 600 MHz.

Fluorohydrin (*cis* and *trans*)

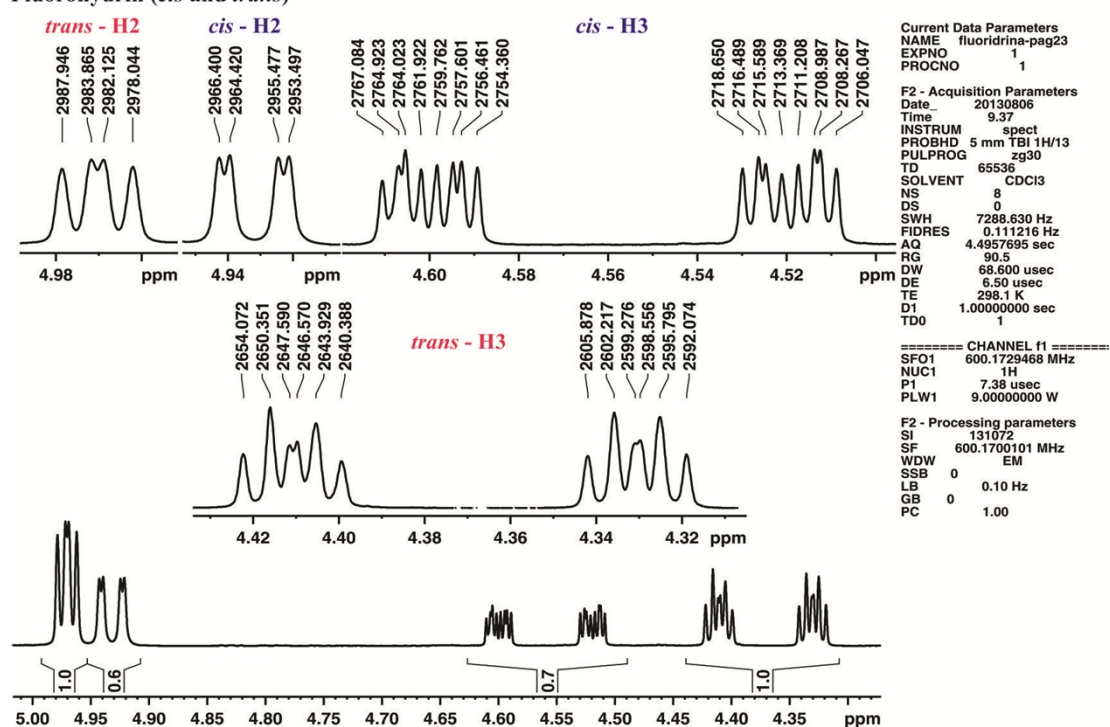


Figure S2: Expansion of ^1H NMR spectrum of fluorohydrin. Signals related to Hydrogens H2 and H3 of both diastereoisomers.

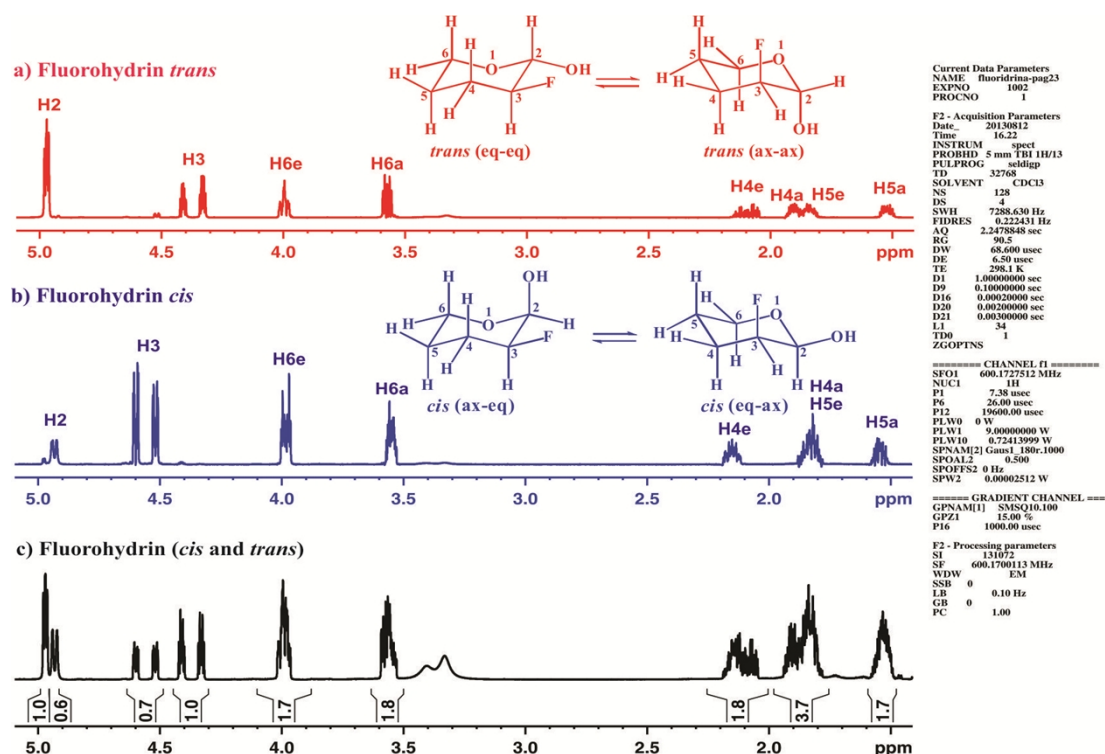


Figure S3: ^1H Sub-spectra with the assignment for fluorohydrin: a) *trans* isomer; b) *cis* isomer acquired through selective TOCSY experiment and c) a normal ^1H NMR spectrum for the *cis* and *trans* mixture.

Chlorohydrin (*cis* and *trans*)

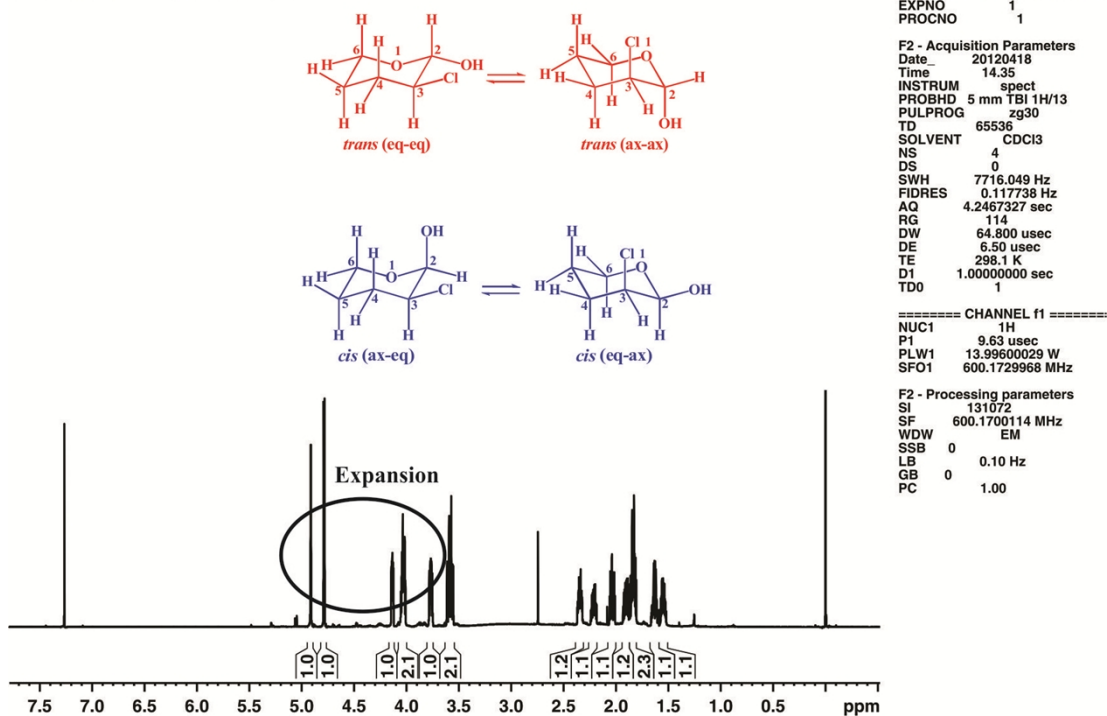


Figure S4: ^1H NMR spectrum of the mixture (*cis* and *trans*) chlorohydrin in CDCl_3 acquired at 600 MHz.

Chlorohydrin (*cis* and *trans*)

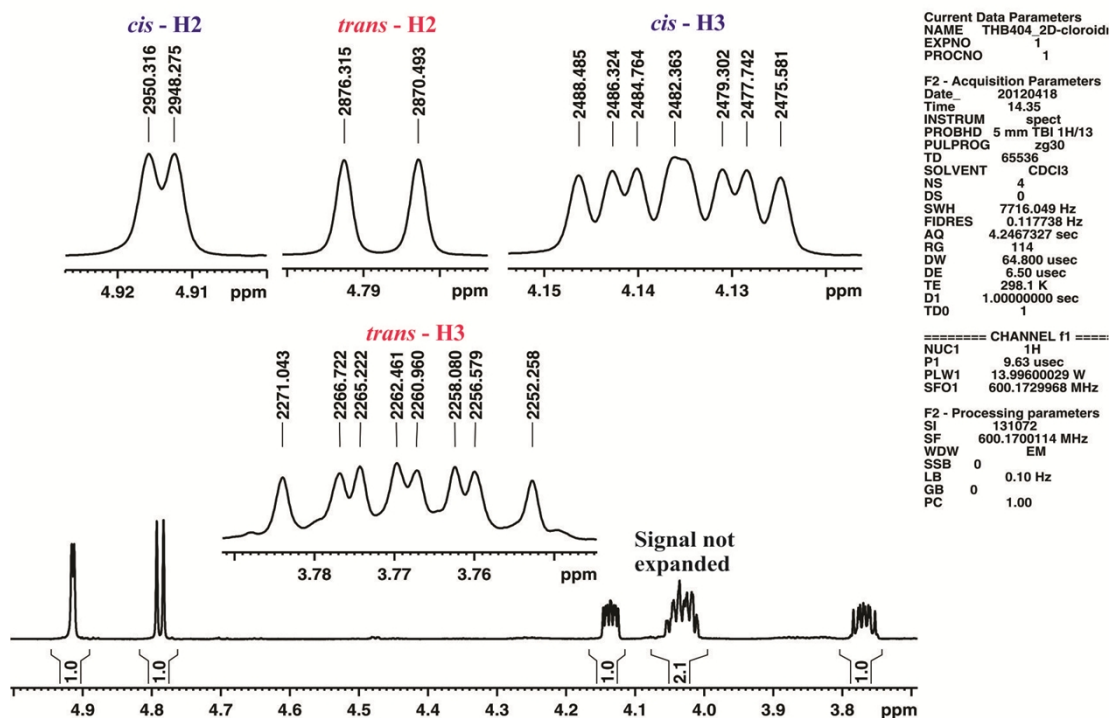


Figure S5: Expansion of ^1H NMR spectrum of chlorohydrin. Signals related to Hydrogens H2 and H3 of both diastereoisomers.

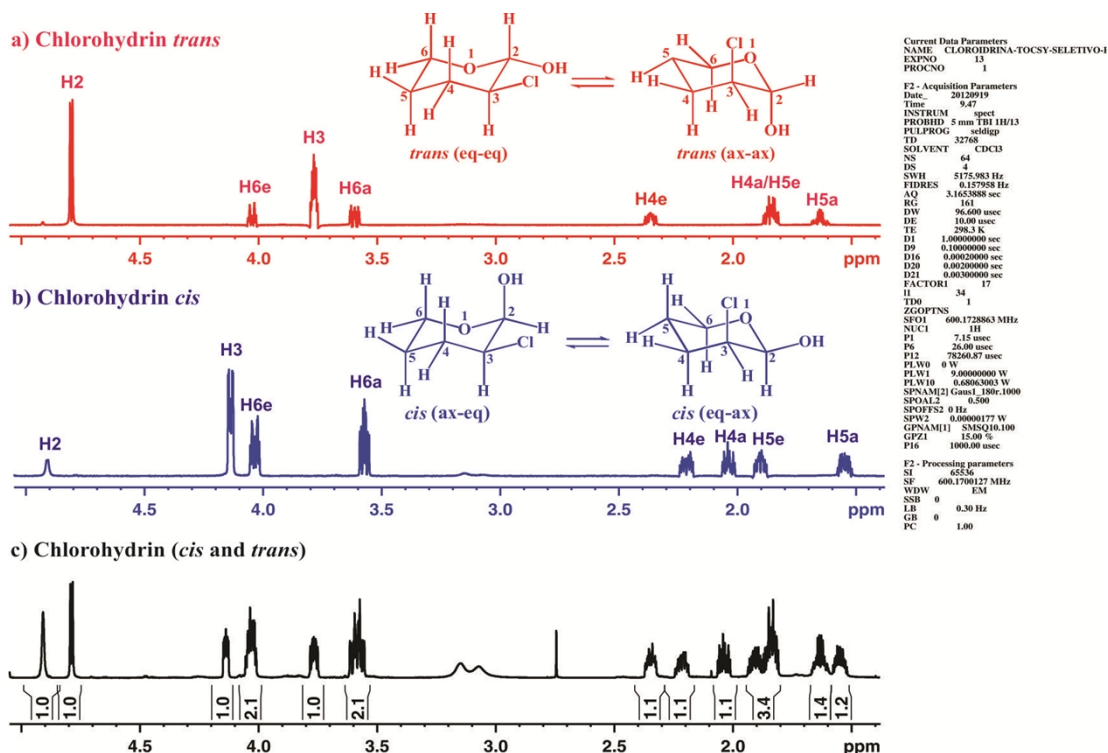


Figure S6: ^1H Sub-spectra with the assignment for chlorohydrin: a) *trans* isomer; b) *cis* isomer acquired through selective TOCSY experiment and c) a normal ^1H NMR spectrum for the *cis* and *trans* mixture.

Bromohydrin (*cis* and *trans*)

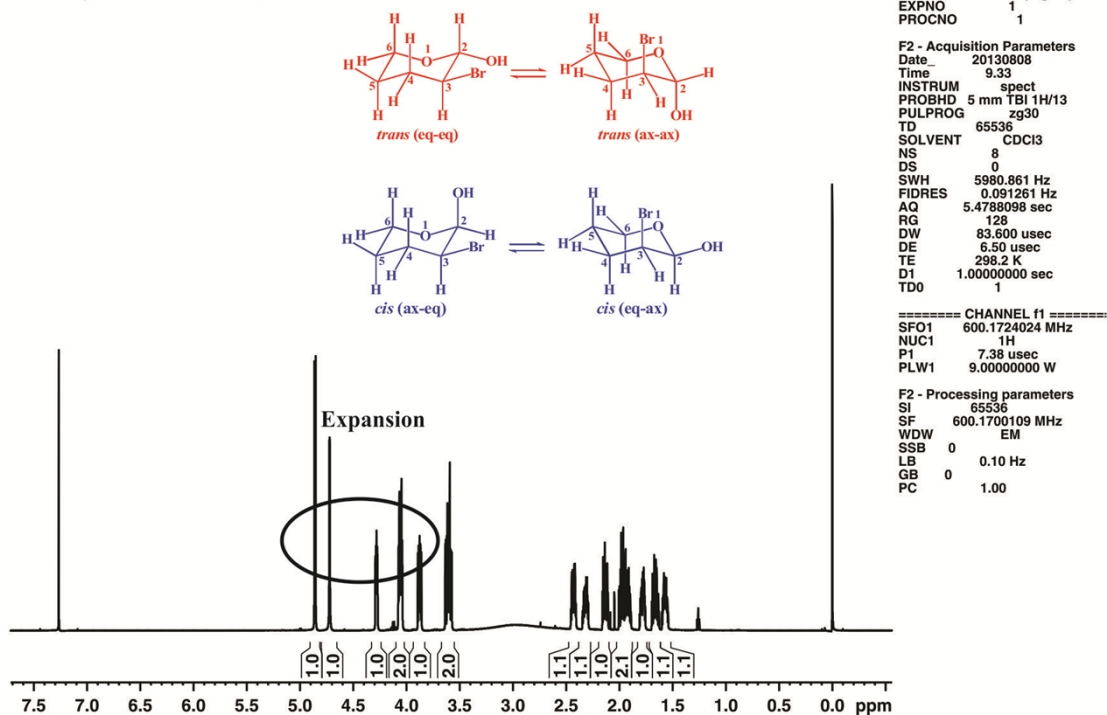


Figure S7: ^1H NMR spectrum of the mixture (*cis* and *trans*) bromohydrin in CDCl_3 acquired at 600 MHz.

Bromohydrin (*cis* and *trans*)

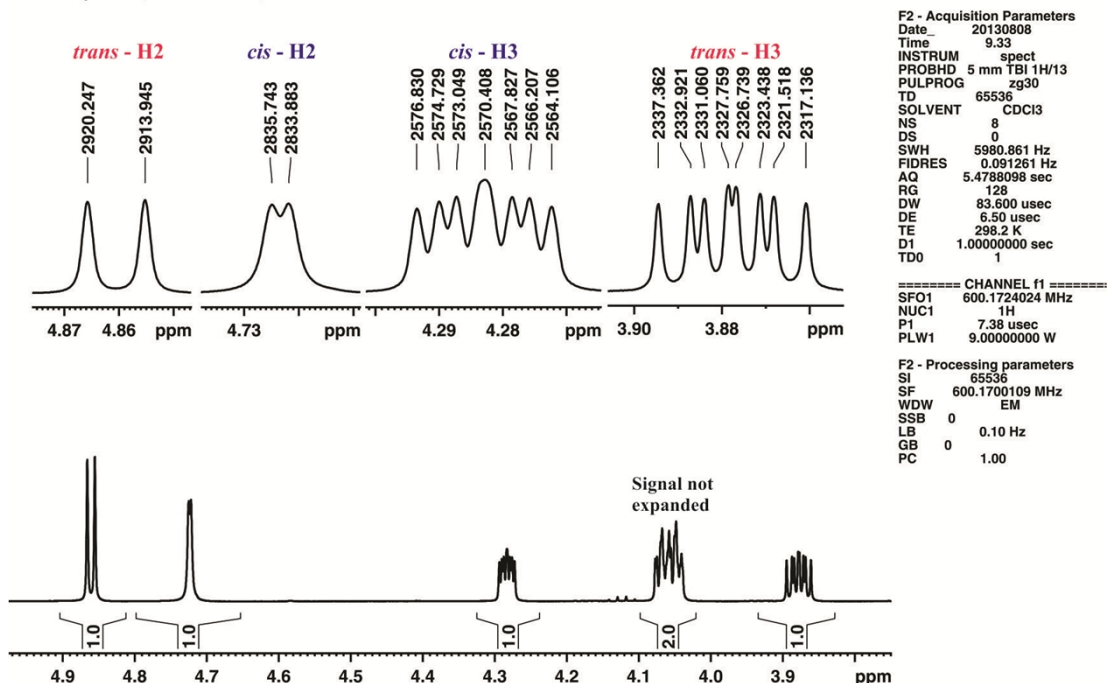


Figure S8: Expansion of ^1H NMR spectrum of bromohydrin. Signals related to Hydrogens H2 and H3 of both diastereoisomers.

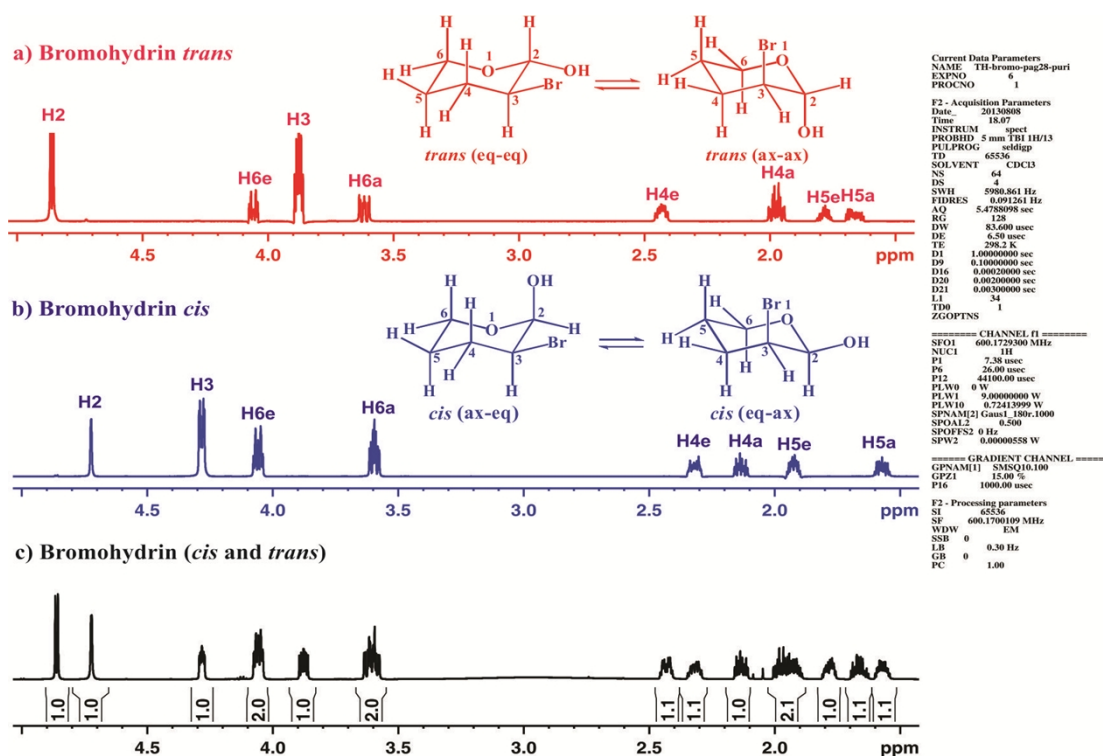


Figure S9: ^1H Sub-spectra with the assignment for bromohydrin: a) *trans* isomer; b) *cis* isomer acquired through selective TOCSY experiment and c) a normal ^1H NMR spectrum for the *cis* and *trans* mixture.

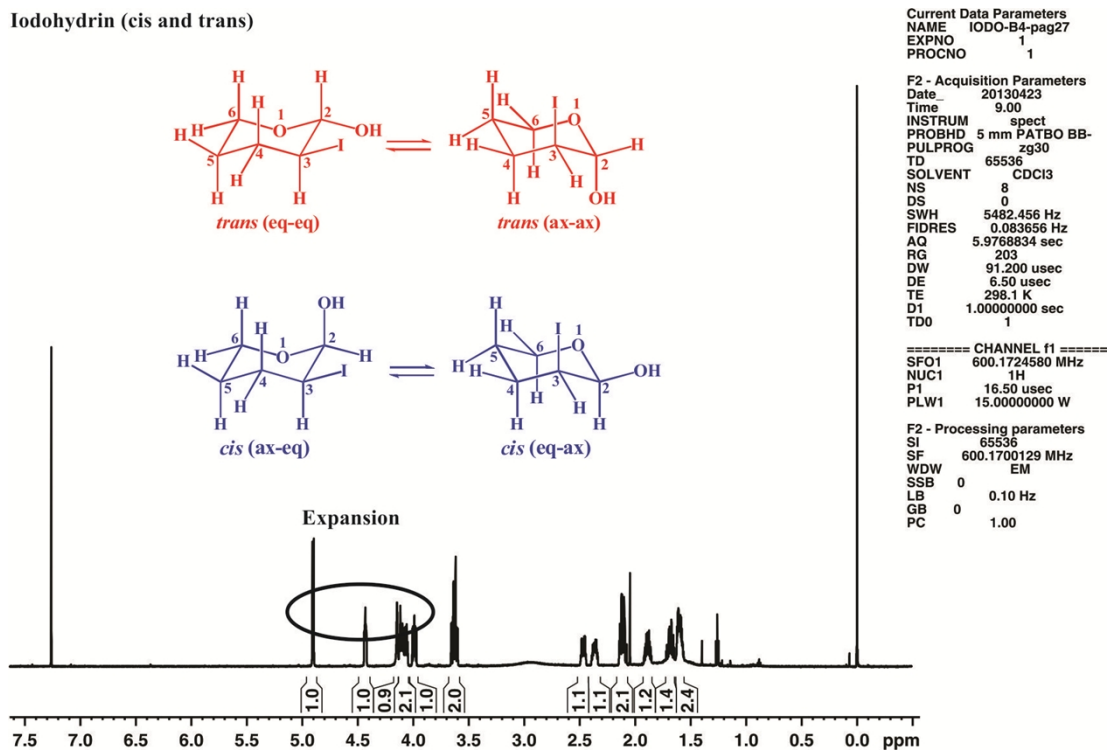


Figure S10: ^1H NMR spectrum of the mixture (*cis* and *trans*) iodohydrin in CDCl_3 acquired at 600 MHz.

Iodohydrin (*cis* and *trans*)

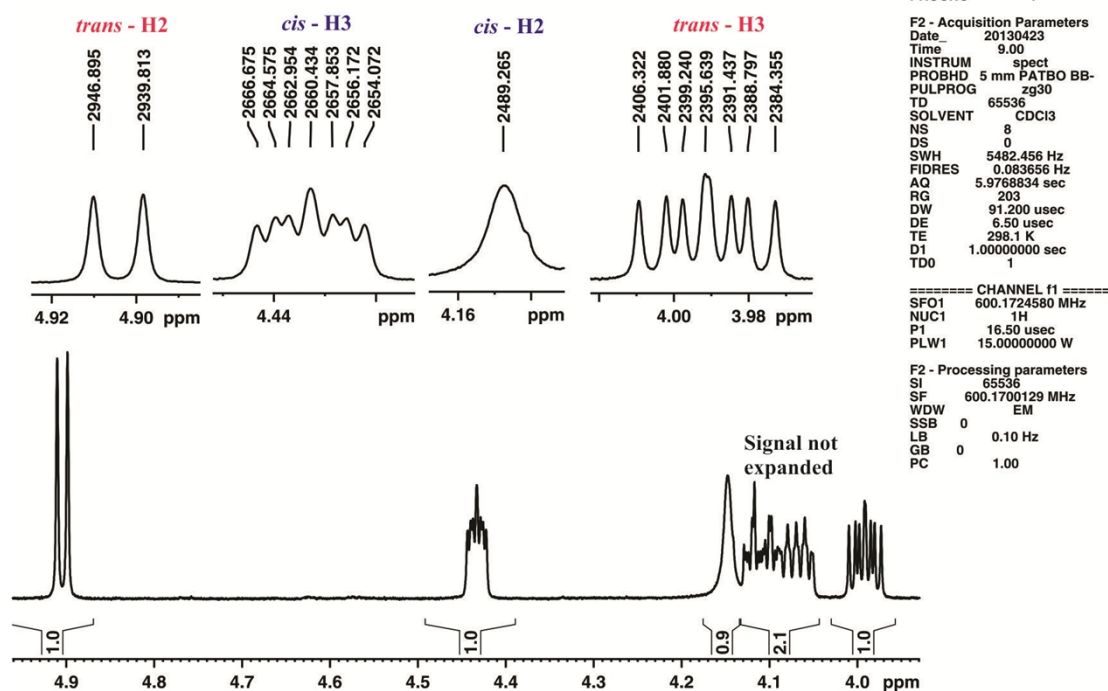


Figure S11: Expansion of ^1H NMR spectrum of iodohydrin. Signals related to Hydrogens H2 and H3 of both diastereoisomers.

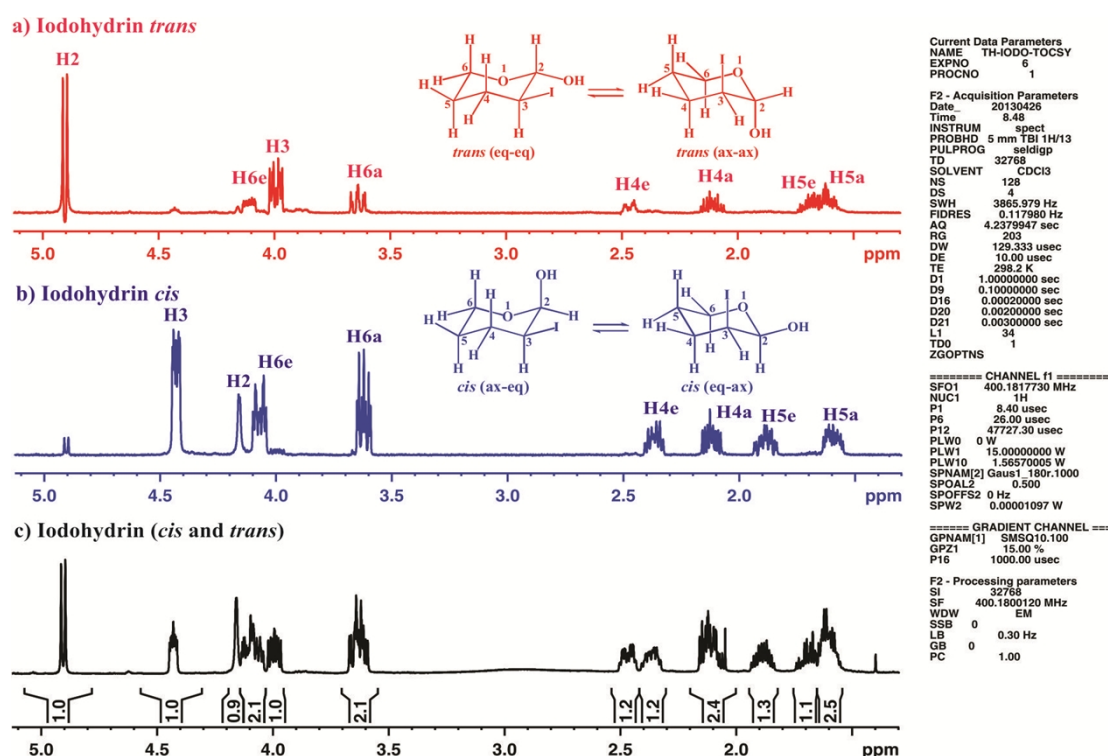


Figure S12: ^1H Sub-spectra with the assignment for iodohydrin: a) *trans* isomer; b) *cis* isomer acquired through selective TOCSY experiment and c) a normal ^1H NMR spectrum for the *cis* and *trans* mixture.