ASSOCIATED CONTENT

SUPPORTING INFORMATION FOR

Towards improved accuracy in chlorine isotope analysis: synthesis routes for in-house standards and characterization via complementary mass spectrometry methods

Christina Lihl[†], Julian Renpenning[∫], Steffen Kümmel[∫], Faina Gelman[‡], Heide K. V. Schürner[†], Martina Daubmeier[†], Benjamin Heckel[∓], Aileen Melsbach[†], Anat Bernstein[§], Orfan Shouakar-Stash[ǁ], Matthias Gehre[∫], Martin Elsner*[†∓]

[†] Institute of Groundwater Ecology, Helmholtz Zentrum München, Ingolstädter Landstraße 1, 85764 Neuherberg, Germany

[∫] Department of Isotope Biogeochemistry, Helmholtz Centre for Environmental Research – UFZ, Permoserstraße 15, 04318 Leipzig, Germany

[‡] Geological Survey of Israel, 32 Yeshayahu Leibowitz St., 9692100 Jerusalem, Israel

[∓] Chair of Analytical Chemistry and Water Chemistry, Technical University of Munich, Marchionistraße 17, 81377 München, Germany

[§] Zuckerberg Institute for Water Research, Department of Environmental Hydrology and Microbiology, Ben-Gurion University of the Negev, 84990 Sede Boqer, Israel

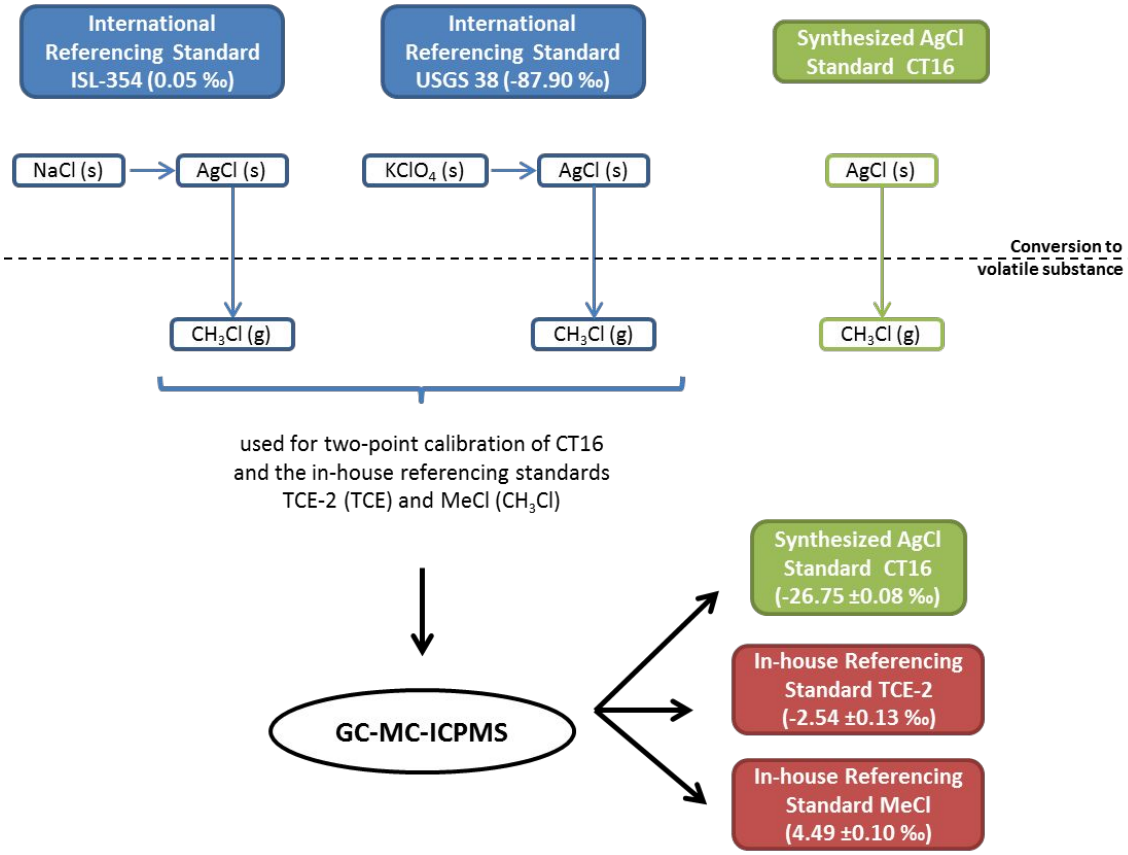
[ǁ] Department of Earth Sciences, University of Waterloo, 200 University Avenue, Waterloo, Ontario, Canada N2L 3G1

* Corresponding Author: Phone: +49 89/2180-78231. E-mail: m.elsner@tum.de

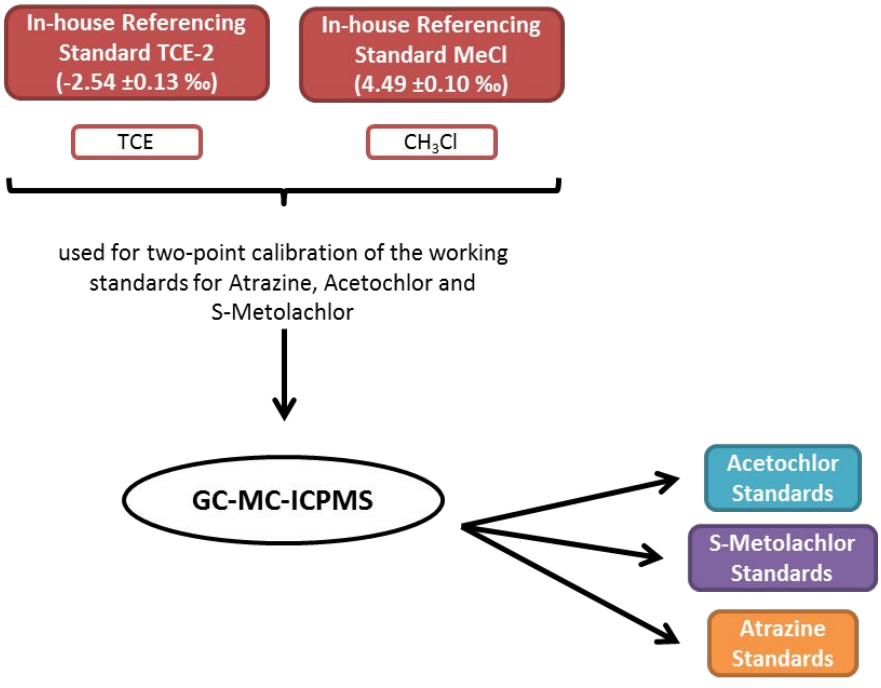
Summary:

3 Pages, 3 Schemes, 1 Table

Scheme S1: Illustrating the workflow of the isotopic characterization of CT16, TCE-2 and MeCl via GC-MC-ICPMS.



Scheme S2: Illustrating the workflow of the isotopic characterization of Atrazine, Acetochlor and S-Metolachlor working standards via GC-MC-ICPMS.



Scheme S3: Illustrating the workflow of the isotopic characterization of CT16 via GC-IRMS.

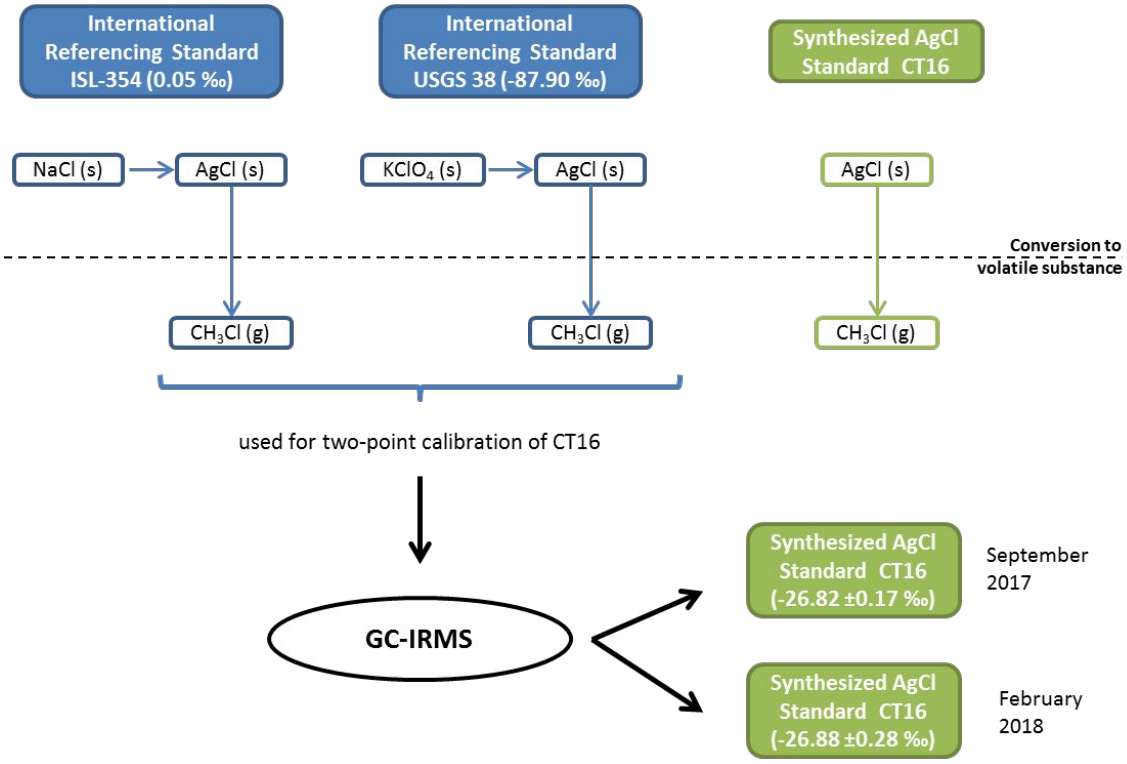


Table S1: List of purchased semi-volatile substances, which were calibrated against the in-house referencing standards TCE-2 and MeCl to be used as working standards in the future.

Working Standard	Substance	Supplier	$\delta^{37}Cl \pm SD^*$ [‰]
ATR #4	Atrazine	Oskar Tropitzsch	-0.89 ± 0.24
ATR #11	Atrazine	Riedel-de Haën	3.59 ± 0.37
ATR_A	Atrazine	Oskar Tropitzsch	-0.89 ± 0.05
ACETO_A	Acetochlor	Chemos	-0.12 ± 0.16
METO_A	S-Metolachlor	Oskar Tropitzsch	-0.01 ± 0.12
METO_B	S-Metolachlor	Chemos	-2.75 ± 0.09

*SD = standard deviation