

Main datasets of "*Simultaneous organic aerosol source apportionment at two Antarctic sites reveals large-scale and eco-region specific components*" by Marco Paglione et al.

Work-sheets:

- **IC&PM1** - reporting the concentrations of Water Soluble Organic Carbon and main other ions as measured by TOC-Analyzer (Shimadzu TOC-5000A) and Ion-Chromatography (IC, Dionex).
 - all the data are concentrations expressed as $\mu\text{g m}^{-3}$
 - the main ions constituting sea-salt are grouped based on the global average sea-salt composition found in Seinfeld&Pandis, 2016 (Seinfeld J.H. and Pandis S.N., Atmospheric chemistry and physics – from air pollution to climate change, Third edition, p354, John Wiley & Sons, New York, 2016)
- **H-NMR_Conc&Contr** - reporting:
 - the functional groups distribution, expressed both in $\mu\text{molH m}^{-3}$ and $\mu\text{gC m}^{-3}$ (using conversion factors described in Decesari et al., 2000 and in the supplementary material of the paper)
 - the concentrations of some molecular tracers (namely Methane-sulphonic acid (MSA), Di- and Tri- methyl amines (DMA and TMA)), expressed in ng m^{-3}
 - the contributions of the factors resulting from the Factor analyses of H-NMR spectral dataset, expressed in $\mu\text{molH m}^{-3}$
- **H-NMR_AmbSpectra** - reporting the full resolution H-NMR spectra of ambient PM1 collected at Signy and Halley.
 - the spectra are aligned all together and truncated to remove the interferent signals from solvent (H_2O signal around 4.9ppm), of the buffer (around 8.45ppm) and the extremes (>9 and $< 0.5\text{ppm}$)
 - in particular all the signal >9 , comprised between 8.61 $<$ 8.15, between 4.9 $<$ 4.65 and <0.5 are removed
- **H-NMR_FA_Profiles** - reporting the spectral profiles of the factors resulting from the Factor analyses of H-NMR dataset, expressed in $\mu\text{molH m}^{-3}$.
 - the original spectra are binned every 40 points (corresponding to 0.02ppm) before the statistical analysis in order to have about 400 final chemical shifts
 - in particular, 2 different solutions are reported from the two different algorithm used:
 - ME2, applying the PMF method using Multilinear-engine solver by Paatero et al. (1999)
 - MCR, i.e., applying the Multi Curve Resolution - Alternating Least Square algorithm by Jaumot et al. (2005) and Tauler (1995)
 - and the mean values between the two.
- **H-NMR_FA_Raw_input** - reporting the input matrixes used for the non-negative factor analysis. Here are reported both the data matrix (named "Data") and the uncertainty matrix ("Unc", necessary to run the PMF using the ME2 algorithm). Uncertainty/error matrix is calculated from the signal-to-noise ratios of the NMR spectra, as already described in previous publications cited in the paper (Decesari et al., 2011; Finessi et al., 2012; Paglione et al., 2014a)