

427 Prioritization, screening and identification of organosilicon contaminants in the environment A.H. Kierkegaard, M.S.

McLachlan, Stockholm University; K. Breivik, Norwegian Inst for Air Research; J.A. Arnot, ARC Arnot Research Consulting / Department of Physical Environmental Science; F. Wania, University of Toronto at Scarborough / Department of Physical & Environmental Sciences. A mass balance model of chemical fate and bioaccumulation in the environment was used to rank 287 high- and low-production volume organosilicon compounds for their concentration in the environment and in top predators. Key physical chemical properties of each chemical were estimated using quantitative structure-activity relationships (QSARs) and a total emission estimate of each chemical was made using information, which included amounts entering commerce and emission factors. Based on the model predicted concentrations in air, sediment and human tissue, chemicals were selected for screening through environmental sampling and analysis. Known environmental organosilicon contaminants such as the cyclic and linear volatile methyl siloxanes (VMS) were excluded as well as structures subject to rapid hydrolysis, a feature which was not taken into account in the model simulations because of current limitations in predicting hydrolysis half-lives with QSARs. Analytical standards were only commercially available for half of the remaining 30 organosilicon compounds. Ten of these were not stable in solution, which left 5 organosilicon compounds eligible for environmental screening. These were tetrakis(trimethylsilyloxy)silane, phenyl-tris(trimethylsilyloxy)silane, trifluoropropyltrimethylcyclotrisiloxane, trifluoropropylmethylcyclotetrasiloxane and tetraphenyltrisiloxane. Four of these chemicals were identified in sewage sludge, in sediment from Stockholm harbor, and in Stockholm ambient air samples. The trifluoropropyl-substituted siloxanes were analysed with UPLC-MS/MS, the others with GC-MS. Trifluoropropyltrimethylcyclotrisiloxane was solely detected as its corresponding linear diol. To date it is unclear whether the diol is present in the environment as such or formed during extraction or cleanup. The concentrations of the chemicals ranged from pg m^{-3} in air up to ng g^{-1} d.w. in sewage sludge, which are orders of magnitude below the levels of cyclic VMS (such as D5) in the same matrices.