Thesis title: Environmental Levels of PAHs and Other SVOCs in a Petrochemical Area. Combining Monitoring and Modelling Tools

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In this thesis atmospheric pollution due to the presence of semi-volatile organic compounds (SVOCs) has been assessed in Tarragona country Spain, where one of the largest chemical/ petrochemical complex in Southern Europe is located. Among these contaminants there are the polycyclic aromatic hydrocarbons (PAHs), compounds mostly emitted by anthropogenic sources, being the oil refineries a considerable emission point. Likewise, pollutants as polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), brominated flame retardants (BFRs) and synthetic musk fragrances (SMs) also have been analysed. Passive Air Sampling techniques such as Passive Air Samples with polyurethane foam (PUF-PAS), lichen transplants, vegetation and soils have been utilised for pollution monitoring. Those techniques can provide information on the contaminants levels at different locations, involving low or no maintenance and reduced costs. Also an extraction method for soils and vegetation based on QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) methodology combined with GC-MS (Gas Chromatography–Mass Spectrometry) have been developed to analyse PAHs, PCBs, HCB, BFRs and SMs.

Results indicate that PUF-PAS mainly capture the pollutants of low molecular weight (most volatile), that are present in gas phase. Concerning to vegetation, results indicate that this matrix capture the pollutants present in the gas phase, but also retains some of them associated to the particulate phase (which has not been washed by natural processes), while soils tend to capture the heaviest, the less volatile and the most resistant to degradation pollutants mainly associated to the particulate phase.

Results obtained have been modelled with MUM-Fate and WRF+CHIMERE models in order to predict PAHs fate, emissions and future concentrations considering actual and future climate conditions (RCP8.5 scenario, 2031-2050). Predictions indicate that concentrations of Benzo(a)pyrene will increase in air and decrease in soils, resulting in an increase of 5x10-8 in the life-time risk of lung cancer, particularly in the most populated areas.