Supplementary Information to

The application of isotopically labelled analogues for the determination of small organic compounds by GC/MS with selected ion monitoring

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Figure S1. Fragments of total ion currents (TICs) with extracted selected ion chromatograms (magnitude x50) of m/z values of selected targets; for example the TIC chromatogram of IBU-SILS peak with extracted SIM chromatogram of 160, 117, 234, 263 m/z belonging to IBU

Figure S2. Change of the quantifier/qualifier ratios (%) (m/z values specified in the brackets) for tested analytes with increasing of the EI ion source temperature

Figure S3. The selected values of quantifier/qualifier ratios

Figure S4. The fragment of SIM chromatogram of IBU, DIC and BPA detected in treated and raw wastewater

Section S1. Guidelines for SIM ions selection with special remarks for silyl derivatives and ILS method



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Figure S2. Change of the quantifier/qualifier ratio (%) (m/z values specified in the brackets) for tested analytes with increasing of the EI ion source temperature



Figure S3. The selected values of quantifier/qualifier ions ratio (%) for analytes with decreasing of analytes concentrations (4.0000 to 0.0164 μ g/mL)



Figure S4. The fragment of SIM chromatogram of IBU, DIC and BPA detected in treated and raw wastewater

Section S1. Guidelines for SIM ions selection for silyl derivatives of targets and SILISs:

- The m/z of common contamination in GC and peaks of background (like leaks of septum, stationary phases) should be avoid.

- The quantifier and qualifier should be taken from characteristic ions with the highest intensity. The use of ions m/z 73 (TMS group) as the qualifier is not recommended. Taken the mass with lower than m/z 200 increase the problem with ratio in real samples.

- The protocol of ratio tolerance should be used and specified in report.

- The overlapping of the peaks from analytes and internal standards, even if the isotopically labelled standards are used, should be checked.

- The molecular ions is valuable ion for SIM, if it have sufficient intensity.