

Table 1.

ESI	Negative Mode
m/z for IS	212.100 → 81.0800
m/z for PCS	187.0500→107.0000
Nebulizing Gas Flow	3 L/min
Drying Gas Flow	15 L/min
DL Temperature	250 °C
Heat Block Temperature	400 °C
Flow	0.5 ml/min
Mobile Phase A	H ₂ O + 0.1% Formic Acid
Mobile Phase B	Acetonitrile
Injection Volume	5 µL
Column Temperature	40°C
Solvent Gradient	Binary Gradient (B): 0 min 1%, 1 min 1%, 6.5 min 65%, 6.6 min 90%, 8 min 90%, 8.1 min 1% for equilibration until 10 min.

Table 1. Operating conditions for the determination of pCS and IS via LC-MS. The table shows all the analytical condition for the analysis, as well as the detection of the UTs. The mass analyser is a triple quadrupole.

Table 2.

Detection Wavelength	200 nm
Mobile Phase A	H ₂ O
Mobile Phase B	Acetonitrile
Flow	0.5 mL/min
Column Temperature	25 °C
Injection Volume	5 µL
Solvent Gradient	30% of B for the duration of the run

Table 2. Operating conditions for the determination of pCS and IS via HPLC-UV. The analysis is carried out in isocratic mode (% of B remains the same for the duration of the run) in reversed phase. The detection is carried out at 200 nm.

Table 3.

Indossyl Sulphate Calibration		
Level	Concentration	STD Mean
1	0,003125	1636524
2	0,00625	1707691
4	0,025	3047901
5	0,05	4670591
sample 1	0,05	17939145
sample 2	0,075	25803228
sample 3	0,1	29569019
sample 4	0,125	37286587
sample 5	0,175	56369180

Table 3. Data referring to the 4-point calibration of IS and the diluted samples 1-5. The operator diluted the samples following the aforementioned ratios and the analysis was carried out at the same operating conditions as the calibration.

Table 4.

P-Cresol Sulphate Calibration		
Level	Concentration	Mean Area
1	0,003125	21211021
2	0,00625	22476552
4	0,025	38158732
5	0,05	60826331
sample 1	0,05	90409199
sample 2	0,0333	1,1E+08
sample 3	0,025	1,29E+08
sample 4	0,02	1,44E+08
sample 5	0,014	1,3E+08

Table 4. Data referring to the 4-point calibration of pCS and the diluted samples 1-5. The operator diluted the samples following the aforementioned ratios and the analysis was carried out at the same operating conditions as the calibration.