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A NOVEL STRATEGY TO RAPID CHARACTERIZATION AND QUANTIFICATION OF COMMERCIAL POLYSORBATE 80 BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY WITH QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY AND COMPUTER-AIDED DATA ANALYSIS

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Polysorbate 80, as a nonionic surfactant with high surface activity and low toxicity, is widely used in the pharmaceutical, personal care and food industries. However, due to its complexity of composition and similarity of compound skeleton, it is difficult to be analyzed rapidly and comprehensively. In this work, a novel strategy was developed to characterize and quantify the commercial polysorbate 80 by high performance liquid chromatography with quadrupole time-of-flight mass spectrometry (HPLC-Q/TOF MS) and computer-aided data analysis. Firstly, a HPLC-Q/TOFMS method was established, and 143 compounds of 7 main high abundance groups in polysorbate 80 were discovered and identified, including: polyethylene oxide(PEO)- sorbitan, PEO-isosorbitan, PEO-sorbitanmonooleate, PEO-isosorbitan-monooleate, PEO-sorbitan-dioleate, PEO-isosorbitan-dioleate, positional isomers of PEO-sorbitandioleate and PEO-sorbitan-trioleate. Then their structures were further confirmed by 1H-NMR and 13C-NMR technology. In addition, 55 trace components in the polysorbate 80 were also identified, including: PEO, PEO-monooleate, PEO-sorbitan-monolinoleate, PEO-sorbitan-monostearate and PEO-sorbitan-monopalmitate. Secondly, colligative properties between the precise molecular weight and retention time of compounds in each group were found. Using these properties, compounds can be rapidly and accurately categorized and calculated the polymerization degree of PEO. Lastly, an automatic identification software of polysorbate 80 based on the above results was developed. After importing the LC-MS data into this software, compounds in commercial polysorbate 80 samples can be identified by molecular weight and retention time, further confirmed by fragment ions and relatively quantified by peak area, realizing rapid, accurate and comprehensive qualitative and quantitative analysis.

Biography

Zhe Wang is a research assistant in Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College. He has engaged in the research of pharmacuetical analysis and drug metabolism since 2009, including drug metabonomics, drug metabolic flux analysis, pharmacokinetics, drug metabolites discovery and identification, illegal adulterants detection in health foods, doping control. He has published 6 papers (first author), including: Journal of Chromatography B, 2017, 1040: 250; Phytomedicine, 2016, 23: 621; Journal of Separation Science, 2015, 38: 925, etc. Research interests are analytical method and strategy for discovery, identification and determination of target multiple compounds in complex matrix samples, such as plasma, urine and herbal medcine, using different effective separation techniques.

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