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On-line/real time compatibility of COBAC analysis, QSPR, QSAR and SBGN big data mining as a novel tool for physiochemical prognostics in the biomedicine-assisted screening and experimental toxicology and allergology

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A current global trend in the development of biomedical and pharmaceutical chemistry is the use of computerized analytical technologies like COBAC, typically followed by the comparison with the action of the known alalytes using QSAR/QSPR methods. The clinicians are interested not in the results of the primary measurements, but in representative results of the physiological and biochemical tests compared with the preceding drugs and their analogs. In this case, a direct conversion of numerical data into the QSAR/QSPR descriptor values with their subsequent transformation to the qualimetric results is necessary, which is described in this paper.

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Notes:

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