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Design of microfluidic devices for fast determination of octanol/water partition coefficients by HPLC

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The estimation of partition coefficients (*P*) is a valuable approach for knowing the performance of bioactive compounds in biological and natural environments. Nevertheless, traditional "shake-flask" techniques for establishing the octanol-water partition coefficient ($P_{o/w}$) are static, time-consuming, and require important volumes of solvents and reagents. To solve these issues, two dynamic microfluidic devices have been designed and created. They have a 3D structure with two independent microfluidic channels, where the octanol (O) channel flows above and perpendicularly through the water (W) channel, allowing for continuous and bi-directional perfusion of the W/O solution. By tilting the devices, flow is completed via the connected microfluidic channels. The devices are integrated into HPLC sampling microplates for direct injection into the instrument. The particular designs and technique allow faster equilibration times, lower consumption of reagents, and can be easily automated, making it appropriate for standard laboratory use. In this presentation, the performance of the designed microfluidic chips is tested by measurement of the log $P_{o/w}$ of some well-known pharmaceutical drugs.