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Measurement of diffusion coefficients of parabens and steroids in water and 1-octanol

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By using the chromatographic broadening method, diffusion coefficients (D) of parabens and steroids in water and 1-octanol were determined at 37 °C, and the relationships between the D values and the physicochemical properties of the drugs were discussed. The D values in 1-octanol were lower than those in water because of the higher viscosity of 1-octanol. The D values depend on not only the molecular weight (MW), but also the lipophilicity of the drugs in water and on the ability for hydrogen-bonding in 1-octanol. When the lipophilic index (LI), calculated from the retention time using in a reverse-phase column, was used as a parameter of drug lipophilicity, the following equation was obtained for D in water (D_w); $\log D_w = -0.215 \log MW - 0.077 \log LI - 4.367$. When the hydrogen bond index (HI), the logarithm of the ratio of the partition coefficient of the drugs in 1-octanol and cyclohexane, was used as an index of hydrogen-bonding, the following equation was obtained for D in 1-octanol (D_o); $\log D_o = -0.690 \log MW - 0.074 \log HI - 4.085$.