

S4 Supporting information. LogD calculation.

Software name and version: ACD/Percepta 14.0.0 (Build 2726)

Compound name: DR5026

LogD at:

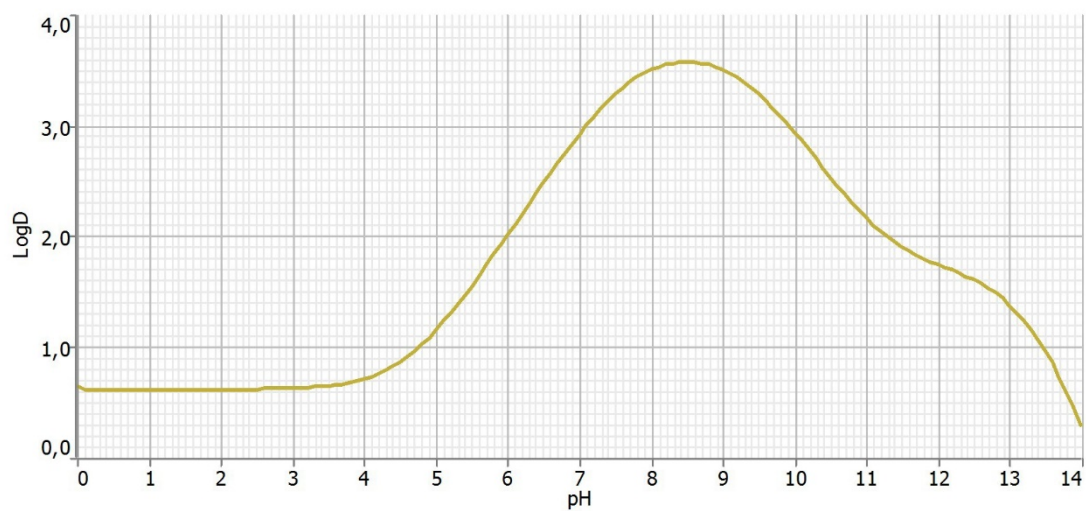
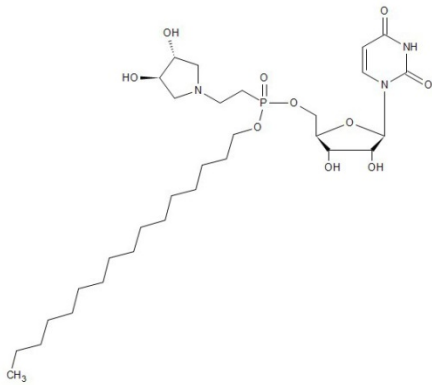
pH = 1,7 (Stomach): 0,61

pH = 4,6 (Duodenum): 0,91

pH = 6,5 (Jejunum and Ileum): 2,48

pH = 7,4 (Blood): 3,22

pH = 8,0 (Colon): 3,51



Compound name: DR5047

LogD at:

pH = 1,7 (Stomach): 0,73

pH = 4,6 (Duodenum): 1,03

pH = 6,5 (Jejunum and Ileum): 2,62

pH = 7,4 (Blood): 3,35

pH = 8,0 (Colon): 3,63

