Supporting Information

CycPeptMPDB: A Comprehensive Database of Membrane Permeability of Cyclic Peptides

Jianan Li[1], Keisuke Yanagisawa[1, 2], Masatake Sugita[1, 2], Takuya Fujie[1, 2], Masahito Ohue[1, 2], and Yutaka Akiyama[1, 2, *]

1. Department of Computer Science, School of Computing, Tokyo Institute of Technology, Meguro-ku, Tokyo 152-8550, Japan
2. Middle-Molecule IT-based Drug Discovery Laboratory (MIDL), Tokyo Institute of Technology, Meguro-ku, Tokyo 152-8550, Japan

* To whom correspondence should be addressed.
Contact: akiyama@c.titech.ac.jp

1 Supplemental Tables

Table S1: Source literature list for CycPeptMPDB. The number of peptides, molecular weight range, and assay type of membrane permeability for each source are shown.

Source	Peptides	Molecular weight	PAMPA	Caco-2	RRCK	MDCK
2006_Rezai_1 [1]	10	712.9 – 1202.6	√			
2006_Rezai_2 [2]	11	710.9 – 840.1	√			
2011_White [3]	10	712.9 – 1202.6			√	
2012_Rand [4]	16	712.9 – 828.1		√	√	
2013_CHUGAI [5]	878	813.0 – 1777.7	√			
2013_Zaretsky [6]	2	471.6 – 627.8		√		
2014_Nielsen [7]	4	709.9 – 778.0			√	
2015_Ahlbach [8]	34	414.5 – 1620.7	√			
2015_Bockus_1 [9]	16	755.0 – 1202.6	√		√	
2015_Bockus_2 [10]	17	707.9 – 778.0	√	√		
2015_Hewitt [11]	18	712.9 – 755.0		√		
2015_Lewis [12]	2	712.9 – 755.0	√			√
2015_Marelli [13]	10	454.5 – 849.0	√	√		
2015_Nielsen [14]	3	724.9 – 785.1	√			
2015_Schwochert [15]	13	712.9 – 793.0			√	
2015_Wang [16]	62	454.5 – 882.1	√	√		
2016_Fouché [17]	15	790.9 – 1199.6				√
2016_Frost [18]	12	542.6 – 699.9	√			
2016_Furukawa [19]	688	606.8 – 944.2	√	√		
2016_Hickey [20]	18	662.8 – 1202.6	√			
2016_Schwochert [21]	8	696.9 – 731.0				√
2017_Boehm [22]	14	848.1 – 929.1			√	
2017_Price [23]	2	1019.4 – 1202.6			√	
2017_Pye [24]	21	785.0 – 1151.5	√		√	
2018_Buckton [25]	19	596.7 – 744.8	√	√		
2018_CHUGAI [26]	374	1062.3 – 1664.2		√		
2018_García-Pindado [27]	4	725.9 – 883.7	√			
2018_Kaneda [28]	7	842.1 – 870.1	√			
2018_Lee [29]	6	639.7 – 653.7	√			
2018_Naylor [30]	81	578.8 – 1218.6	√		√	
2018_Ramalho [31]	10	767.0 – 851.0	√	√		
2019_Ono [32]	8	712.9 – 712.9	√			
2020_Barlow [33]	26	537.7 – 753.0	√			
2020_Furukawa [34]	36	987.3 – 1197.5	√			√
2020_Hosono [35]	11	712.9 – 727.0	√			
2020_Le Roux [36]	47	342.4 – 486.7	√	√		
2020_Townsend [37]	3086	654.9 – 958.2	√			
2021_Comeau [38]	42	430.5 – 458.6	√	√		
2021_Golosov [39]	27	758.0 – 1076.5	√		√	
2021_Kelly [40]	1519	974.3 – 1220.4	√			√
2021_Lee [41]	5	1160.6 – 1231.7	√	√		
2021_Wang [42]	24	959.2 – 1169.5	√			
2022_Bhardwaj [43]	136	622.8 – 1299.7	√	√		
2022_Lee [44]	24	1160.6 – 1251.7	√			
2022_Saunders [45]	11	542.6 – 623.7	√			
2022_Taechalertpaisarn [46]	52	661.8 – 856.1	√			
2022_Tamura [47]	12	792.0 – 950.2	√			

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