

High-throughput measurement of drug-cyclodextrin kinetic rate constants by small molecule microarray using surface plasmon resonance imaging

Vikramjeet Singh^{a,b}, Zhuo Li^{a,c}, Xiaotong Zhou^a, Xiaonan Xu^a, Jianghui Xu^a, Amita Nand^b, Huajie Wen^d, Haiyan Li^a, Jingsong Zhu^{b,d,*}, Jiwen Zhang^{a,*}

^aCenter for Drug Delivery Systems, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China.

^bNational Center for Nanoscience and technology, Beijing, 100190, China.

^cSchool of Pharmacy, Shenyang Pharmaceutical University, Shenyang 110016, China

^dGuangzhou Gaotong Biological Technology Co. Ltd., Guangzhou, 510663, China

Corresponding author:

Dr. Jiwen Zhang

Center for Drug Delivery Systems, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China.

Email: jwzhang@simm.ac.cn

Telephone and Fax: +86-(21)-20231980

Table S-1: The calculated equilibrium association rate constants (KA) obtained from SPRi.

Drug	α- CD	β-CD	γ-CD	HP-β-CD	SBE-β-CD
Glyburide	1.15e8	1.51e8	6.68e8	4.11e8	3.68e7
Glipizide	1.18e8	5.72e8	4.58e8	2.26e8	2.65e8
Silymarin	8.52e7		3.41e6	1.84e8	1.31e7
Captopril	3.73e8	5.28e8	3.01e8	7.12e8	3.72e8
Melatonin	8.45e8	1.3e7	8.6e6	2.87e8	1.09e8
Enalapril	1.17e8	3.91e7	1.28e7	8.64e7	2.46e8
Sunitinib	1.61e7	6.06e7	1.47e7	1.85e7	8.68e7
Ethionamide	1.92e7	8.59e8	3.3e7	1.17e7	1.44e7
Fenbufen	2.52e6	0.253	2.95e7	2.04e7	5.49e7
Phenacetin	5.29e7	1e8	1.79e8	1.03e8	9.7e7
Artemether	3.51e8	2.27e8	1.1e8	3.41e8	2.7e8
Salicylic acid	9.97e7	2.52e8	3.88e7	1.4e8	2.65e8
Theophylline	1.04e7	2.87e8	7.78e9	5.02e8	1.07e8
Paclitaxel	1.55e8	3.15e8	3.11e7	2.21e7	2.03e8
Docetaxel	3.28e8	4.3e7	2.83e7	8.87e8	2.89e7
Dihydroartemisinin	4.76e7	4.09e8	3.06e8	1.85e8	1.27e8
Budesonide	1.18e7	5.38e7	2.62e6	9.99e7	9.04e7
Diclofenac	3.42e8	1.38e8	4.19e7	4.51e6	4.6e6
Flurbiprofen	1.19e6	4.85e7	1.06e8	1.73e8	1.55e8
Caffeine	1.64e8	2.76e7	4.99e7	1.51e8	8.53e7
Metronidazole	1.05e8	2.5e5	4.3e7	8.3e6	4.35e7
Paracetamol	1.34e7	9.59e8	1.6e8	2.54e8	1.7e8
Acyclovir	1.27e8	1.33e8	1.53e8	2.72e8	1.3e8
Fluconazole	6.42e8	3.64e7	8.02e7	4.27e8	3.6e6
Clenbuterol	1.73e8	5.22e8	3.29e8	3.89e8	1.72e8
Trimethoprim	6.04e8	2.74e7	2.25e8	7.04e8	7.57e7
Diazepam	6.35e7	3.28e8	9.06e7	5.44e8	4.43e8
Artemisinin	2.06e8	1.72e7	3.59e7	2.94e7	5.92e7
Nifedipine	9.57e7	1.3e7	1.97e7	9.44e5	2.55e6
Indapamide	1.11e7	2e9	3.34e6	3.42e7	5.36e7
Granisetron	2.77e8	4.19e8	4.28e7	3.04e7	8.6e7
Tolbutamide	1.66e6	3.36e8	1.91e6	1.09e8	8.62e7
Diphenhydramine	2.75e7	5.61e6	6.42e7	2.85e7	2.12e7
Ketoprofen	3.83e8	1.23e8	9.74e7	2.08e8	1.36e6
Piroxicam	2.49e6	9.42e7	4.77e8	1.17e8	2.12e8
Pseudolaric Acid B	5.61e8	1.88e8	1.04e7	2.25e8	1.46e7
Prednisolone	1.05e8	1.28e8	1.41e8	1.99e8	1.2e8
Meloxicam	4.48e8		1.72e8	4.88e7	1.06e8

Table S-2: The calculated dissociation rate constants (k_d) obtained from SPRi.

Drug	α -CD	β -CD	γ -CD	HP- β -CD	SBE- β -CD
Glyburide	1.56e-5	1.05e-5	2.69e-6	1.59e-5	2.57e-5
Glipizide	1.58e-5	1.05e-6	9.74e-6	3.17e-5	1.54e-5
Silymarin	5.86e-7	--	2.16e-5	3.56e-5	2.03e-6
Captopril	9.63e-7	5.45e-6	9.44e-6	1.29e-5	7.95e-6
Melatonin	6.7e-6	5.39e-6	5.95e-5	2.56e-5	1.87e-5
Enalapril	1.4e-5	3.08e-3	5.12e-5	5.99e-6	6.42e-6
Sunitinib	1.65e-6	1.89e-5	2.85e-5	1.02e-5	5.33e-5
Ethionamide	9.64e-6	6.98e-6	1.87e-5	6.75e-6	2.13e-5
Fenbufen	6.03e-6	2.28e-5	1.99e-5	6.51e-5	4.51e-5
Phenacetin	1.43e-5	1.72e-5	2.51e-5	1.7e-5	2.21e-5
Artemether	5.57e-6	4.5e-6	1.61e-5	1.17e-5	8.68e-6
Salicylic acid	1.62e-5	8.17e-6	2.62e-5	4.12e-5	8.83e-6
Theophylline	5.56e-6	1.27e-5	6.02e-7	1.6e-5	1.67e-5
Paclitaxel	1.23e-5	3.17e-6	2.36e-5	1.08e-7	9.77e-6
Docetaxel	2.39e-5	2.33e-5	2.08e-6	7.66e-6	1.79e-6
Dihydroartemisinin	8.44e-7	1.13e-5	1.08e-5	1.33e-5	1.29e-5
Budesonide	2.26e-6	1.17e-6	7.61e-5	6.05e-6	2.26e-5
Diclofenac	5.11e-6	2.55e-5	1.48e-5	3.16e-5	8.63e-5
Flurbiprofen	2.65e-7	4.69e-5	1.58e-5	1.56e-5	1.15e-5
Caffeine	1.16e-5	1.66e-6	2.97e-5	2.98e-5	2.77e-5
Metronidazole	1.82e-5	3.41e-5	1.53e-5	6.55e-5	2.5e-5
Paracetamol	2.99e-6	7.02e-6	3.81e-5	8.59e-6	3.94e-6
Acyclovir	4.88e-6	6.55e-6	1.32e-5	3.26e-5	1.73e-5
Fluconazole	7.06e-6	1.54e-3	3.49e-7	3.26e-6	1.81e-6
Clenbuterol	1.09e-5	6.11e-6	1.03e-5	1.47e-5	9.64e-6
Trimethoprim	2.55e-6	3.54e-5	2.3e-6	3.14e-6	1.17e-5
Diazepam	6.26e-6	4.51e-6	1.6e-5	6.65e-7	3.57e-6
Artemisinin	4.85e-7	3.85e-6	5.7e-5	1.82e-5	2.68e-5
Nifedipine	1.23e-5	3.41e-5	6.27e-5	9.41e-5	6.34e-5
Indapamide	6.23e-7	3.04e-6	7.95e-6	3.29e-5	2.37e-5
Granisetron	6.33e-6	6.35e-6	3.89e-5	6.98e-5	9.38e-6
Tolbutamide	6.04e-7	9.34e-6	7.17e-5	1.82e-5	4.89e-5
Diphenhydramine	2.03e-6	1.12e-6	5.89e-5	4.3e-5	1.62e-6
Ketoprofen	4.81e-6	1.39e-5	1.54e-5	2.24e-5	4.95e-6
Piroxicam	2.6e-6	9.3e-7	8.02e-6	1.52e-5	1.1e-5
Pseudolaric Acid B	5.26e-6	9.54e-6	4.96e-6	8.56e-6	2.6e-5
Prednisolone	8.35e-6	1.3e-5	2.17e-5	1.01e-5	1.37e-5
Meloxicam	7.85e-6	--	1.13e-5	1.87e-5	1.44e-5