

Electronic supplementary information for

Association Models for Binding of Molecules to Nanostructures

By

Manuel Ahumada,^a Eduardo Lissi,^b Ana Maria Montagut,^a Francisco Valenzuela-Henriquez,^c Natalia L. Pacioni,^{d*} and Emilio I. Alarcon^{a,e*}

^a*Bio-nanomaterials Chemistry and Engineering Laboratory, Division of Cardiac Surgery, University of Ottawa Heart Institute, 40 Ruskin Street, Rm H5229, Ottawa, Canada.*

^b*Laboratorio de Cinética y Fotoquímica, Departamento de Ciencias del Ambiente-Facultad de Química y Biología, Universidad de Santiago de Chile, Avenida Libertador Bernardo O'Higgins 3363, Santiago, Chile.*

^c*Instituto de Matemática, Pontificia Universidad Católica de Valparaíso, Blanco Viel 596, Cerro Barón, Valparaíso, Chile.*

^d*INFIQC-CONICET and Universidad Nacional de Córdoba, Departamento de Química Orgánica-Facultad de Ciencias Químicas. Haya de la Torre y Medina Allende s/n, X5000HUA, Ciudad Universitaria, Córdoba, Argentina.*

^e*Department of Biochemistry, Microbiology, and Immunology, Faculty of Medicine, University of Ottawa, Ottawa, ON K1Y 4W7, Canada.*

Authors to whom correspondence should be addressed:

earcon@ottawaheart.ca (EIA); nataliap@fcq.unc.edu.ar (NLP)

Page S1. This page

Page S2. Table S1: Values of binding constants to HSA

Page S8. References

Table S1. Values of binding constants to HSA. The different column values for K_a correspond to different methods of determination, to more information please refer to original reference.

Solute	K_a (10^4) M^{-1}			Reference
	(1)	(2)	(3)	
(+)-catechin	1.21	1.51	-	1
(-)-epicatechin-3-gallate	6.56	5.85	-	2
(-)-epicatechin-3-gallate-Cu(II)	4.84	4.95	-	2
(-)-epigallocatechin-3-gallate-Cu(II)	11.45	11.62	-	2
1-anthracene sulfonate	13.4	1.2	-	3
1-(4-bromophenyl)-2,4,5-triphenyl-1H-imidazole	3.8	-	-	4
1-(4-bromophenyl)-2-(4-fluorophenyl)-4,5-diphenyl-1H-imidazole	3.7	-	-	4
1-(4-bromophenyl)-4,5-diphenyl-2-(thiophen-2-yl)-1H-imidazol	3.0	-	-	4
2-(2-hydroxy-3-ethoxybenzylidene)-1,3-indanedione	5.5	5.5	-	5
2-carboxyphenoxathiin	11	24	-	6
2-hydroxy-3-nitro-9-	60.8	33.6	-	7

fluorenone				
2-pyridone	3.0	1.0	-	8
2'-deoxyuridine	3.5	3.7	-	9
3-acetyl-4-oxo-6,7-dihidro-12H-indolo-[2,3]-quinolizine	1.9	2.1	-	10
3-pyrazolyl-2-pyrazoline	3.65	3.6	4.4	11
3-pyridone	2.3	0.3	-	8
7-hydroxyflavone	9.44	-	-	12
8-bromoadenosine	0.26	0.34	0.34	13
Acetohexamide	18	13	-	14
ANS	630	71	-	15
ANDR	1.85	-	-	16
Amlopidine	2070	-	-	17
Apigenin	9.85	9.8	450	18
Aspirin	103	-	-	17
Azo-4N	5.7	2.1	-	19
Bis-Azo-4N	6.5	2.8	-	19
Benzoporphyrin derivative	10	-	-	20
Bergenin	1.44	-	-	21
Bioactive pyridazinone	8.4	4.22	11.7	22
Bromsulphalein	0.33	3.3	-	23

Brucine	1.82	1.71	-	24
Butylated hydroxytoluene	0.23	-	-	25
Captopril	0.32	13.8	0.97	26
Chlorpromazine	6.2	4.9	-	14
Cromolyn sodium	2.03	1.19	-	27
Curcumin	20	2.1	-	28
Cyanine dye	20	-	-	29
Dexamethasone	2.5	-	-	30
Di-(2-ethylhexyl) phthalate	5.19	-	-	31
Diclofenac sodium	3.37	-	-	30
Dihydropyrimidinones	2.7	1.45	-	32
Doxepin	0.6	0.97	-	33
Fluoxetine hydrochloride	0.15	0.17	-	34
Furosemide	2.71	-	-	30
Gefitinib	1.7	-	-	35
Gemcitabine hydrochloride	7.9	7.2	-	36
Glidazide	8.0	6.9	-	14
Hesperidine	5.1	-	-	37
Icariin	10.15	4.7	-	38

ICT receptor	65	14.1	-	39
Indometacin	0.91	-	-	40
Irisfloreutin	3.44	3.9	-	41
Isoimperatorin	110	-	-	42
JDC-108	18.5	19.5	-	43
Loureirin B	13.14	7.0	2.78	44
m-nitrophenylfluorone-Mo (VI)	5.4	10.6	-	45
Mangiferin	4.17	3.9	-	46, 47
Mapenterol	0.23	0.27	0.21	48
Methyl blue	25.8	6.5	-	49
Methylene blue	3.6	-	-	50
Midazolan	0.4	3.14	-	51
Mitoxantrone	15.6	3.17	2.4*	52 / * 53
Morin	8.7	15.9	-	54
NADA	19.2	-	-	55
NADB	17.5	-	-	55
NADC	16.7	-	-	55
Naringin	1.47	-	-	56
Nevadensin	97	81	180	57
Nobiletin	5.3	4.8	-	58
Norethindrone	0.33	-	-	59

Norethindrone acetate	0.46	-	-	59
Ozagrel	23.4	-	-	60
Palmatine hydrochloride	8.8	9.9	-	61
Paracetamol	0.3	1.3	1.3	62
Paraquat	3.8	4.8	4.0	63
Pd (III) complexes	1.7	0.03	-	64
Phenosafranin	0.54	-	-	65
Piperine	0.62	-	-	66
Piridine derivative	9.55	-	-	67
Pyrazosulfuron-ethyl	2.69	4.41	3.2	68
Quercitin	31.4	-	-	69
Repaglinide	5.7	-	-	70
Resveratrol	16	-	-	47
Resveratrol hexanoic acid	670	312	-	47
Rose Bengal	26	160	-	71
SBDC	4.6	99	-	72
Scutellarin	7.8	7.6	-	73
Shikonin	13.3	13.0	-	74
Sophoricoside	6.0	-	-	75
Sulpiride	5.46	-	-	76
Tetrandine	1.0	40	-	77

Tolbutamide	11.0	9.0	-	14
Thioridazine HCl	5.0	4.5	-	78
Trans urocanic acid	4.0	-	-	79
Vancomycin	0.61	-	-	80
Verapamil	1.5	1.6	-	14
Vincamine	6.1	-	-	81
Vitamin B12	4.3	69	-	82
Warfarin	24	16	8.42*	14, 83*
Wogonin	19.4	18.7	-	84

References

1. X. Li and S. Wang, *New J. Chem.*, 2015, **39**, 386-395.
2. A. Singha Roy, K. S. Ghosh and S. Dasgupta, *J. Biomol. Struct. Dynam.*, 2013, **31**, 1191-1206.
3. P. Banerjee, S. Ghosh, A. Sarkar and S. C. Bhattacharya, *J. Luminescence*, 2011, **131**, 316-321.
4. Y. Yue, Y. Sun, Q. Dong, R. Liu, X. Yan, Y. Zhang and J. Liu, *Luminescence*, 2016, **31**, 671-681.
5. D. Stan, I. Matei, C. Mihailescu, M. Savin, M. Matache, M. Hillebrand and I. Baci, *Molecules*, 2009, **14**, 1614.
6. A. Varlan and M. Hillebrand, *Molecules*, 2010, **15**, 3905-3919.
7. H. Gao, L. Lei, J. Liu, Q. Kong, X. Chen and Z. Hu, *J. Photochem. Photobiol. A: Chemistry*, 2004, **167**, 213-221.
8. O. K. Abou-Zied and O. I. Al-Shihi, *J. Am. Chem. Soc.*, 2008, **130**, 10793-10801.
9. F. Cui, Y. Yan, Q. Zhang, J. Du, X. Yao, G. Qu and Y. Lu, *Carbohydrate Res.*, 2009, **344**, 642-647.
10. P. Das, A. Mallick, B. Haldar, A. Chakrabarty and N. Chattopadhyay, *J. Chem. Sci.*, 2007, **119**, 77-82.
11. P. Banerjee, S. Pramanik, A. Sarkar and S. C. Bhattacharya, *J. Phys. Chem. B*, 2009, **113**, 11429-11436.
12. A. Banerjee, K. Basu and P. K. Sengupta, *J. Photochem. Photobiol. B: Biology*, 2008, **90**, 33-40.
13. F. Cui, Y. Yan, Q. Zhang, X. Yao, G. Qu and Y. Lu, *Spectrochim. Acta Part A*, 2009, **74**, 964-971.
14. X. Zheng, Z. Li, M. I. Podariu and D. S. Hage, *Analytical Chem.*, 2014, **86**, 6454-6460.
15. K. Takehara, K. Yuki, M. Shirasawa, S. Yamasaki and S. Yamada, *Analytical Sci.*, 2009, **25**, 115-120.
16. D. P. Yeggoni, C. Kuehne, A. Rachamallu and R. Subramanyam, *RSC Advances*, 2017, **7**, 5002-5012.
17. N. Abdollahpour, V. Soheili, M. R. Saberi and J. Chamani, *Eur. J. Drug Metab. Pharm.*, 2016, **41**, 705-721.
18. J.-L. Yuan, Z. lv, Z.-G. Liu, Z. Hu and G.-L. Zou, *J. Photochem. Photobiol. A: Chemistry*, 2007, **191**, 104-113.
19. M. Deiana, Z. Pokladek, M. Ziemianek, N. Tarnowicz, P. Mlynarz, M. Samoc and K. Matczyszyn, *RSC Advances*, 2017, **7**, 5912-5919.
20. B. M. Aveline, T. Hasan and R. W. Redmond, *J. Photochem. Photobiol. B: Biology*, 1995, **30**, 161-169.
21. Y. Zhang, L. Dong, Y. Li, J. Li and X. Chen, *J. Fluorescence*, 2008, **18**, 661-670.
22. T. Wang, B. Xiang, Y. Wang, C. Chen, Y. Dong, H. Fang and M. Wang, *Colloids Surf. B*, 2008, **65**, 113-119.
23. F. Q. Cheng, Y. P. Wang, Z. P. Li and C. Dong, *Spectrochim. Acta. Part A*, 2006, **65**, 1144-1147.

24. Y.-Q. Wang, H.-M. Zhang, G.-C. Zhang, W.-H. Tao and S.-H. Tang, *J. Mol. Structure*, 2007, **830**, 40-45.
25. N. A. Al-Shabib, J. M. Khan, M. S. Ali, H. A. Al-Lohedan, M. S. Khan, A. M. Al-Senaidy, F. M. Husain and M. B. Shamsi, *J. Mol. Liquids*, DOI: <http://dx.doi.org/10.1016/j.molliq.2017.01.066>.
26. X. Gao, Y. Tang, W. Rong, X. Zhang, W. Zhao and Y. Zi, *Am. J. Anal. Chem.*, 2011, **2**, 250-257.
27. Y.-J. Hu, Y. Liu, Z.-B. Pi and S.-S. Qu, *Bioor. Med. Chem.*, 2005, **13**, 6609-6614.
28. A. C. Pulla Reddy, E. Sudharshan, A. G. Appu Rao and B. R. Lokesh, *Lipids*, 1999, **34**, 1025-1029.
29. Y.-Z. Zhang, Q.-F. Yang, H.-Y. Du, Y.-L. Tang, G.-Z. Xu and W.-P. Yan, *Chinese J. Chem.*, 2008, **26**, 397-401.
30. Z. J. Yasseen and M. O. El-Ghossain, *J. Biomedical Sci.*, 2016, **5**.
31. Y. Wang and G. Zhang, *Luminescence*, 2015, **30**, 198-206.
32. G. Wang, D. Wang, X. Li and Y. Lu, *Coll. Surf. B*, 2011, **84**, 272-279.
33. P. B. Kandagal, S. Ashoka, J. Seetharamappa, V. Vani and S. M. T. Shaikh, *J. Photochem. Photobiol. A: Chemistry*, 2006, **179**, 161-166.
34. U. Katrahalli, S. Jaldappagari and S. S. Kalanur, *Spectrochim. Acta Part A*, 2010, **75**, 314-319.
35. M. Z. Kabir, W.-V. Tee, S. B. Mohamad, Z. Alias and S. Tayyab, *RSC Advances*, 2016, **6**, 91756-91767.
36. P. B. Kandagal, S. Ashoka, J. Seetharamappa, S. M. T. Shaikh, Y. Jadegoud and O. B. Ijare, *J. Pharm. Biomed. Anal.*, 2006, **41**, 393-399.
37. Y.-Q. Wang, H.-M. Zhang, G.-C. Zhang, W.-H. Tao and S.-H. Tang, *J. Luminescence*, 2007, **126**, 211-218.
38. G. Zhang, Q. Que, J. Pan and J. Guo, *J. Mol. Struct.*, 2008, **881**, 132-138.
39. F.-Y. Wu, Z.-J. Ji, Y.-M. Wu and X.-F. Wan, *Chem. Phys. Lett.*, 2006, **424**, 387-393.
40. E. Mozaffari, E. Tazikeh-lemeski and A. A. Saboury, *Biomacromolecular Journal*, 2016, **2**, 34-43.
41. G. Zhang, A. Wang, T. Jiang and J. Guo, *J. Mol. Struct.*, 2008, **891**, 93-97.
42. S. Ranjbar, Y. Shokoohinia, S. Ghobadi, N. Bijari, S. Gholamzadeh, N. Moradi, M. R. Ashrafi-Kooshk, A. Aghaei and R. Khodarahmi, *Sci. World J.*, 2013, 305081.
43. F. Cui, L. Qin, G. Zhang, X. Liu, X. Yao and B. Lei, *Bioorg. Med. Chem.*, 2008, **16**, 7615-7621.
44. Y. Zhang, Y. Sha, K. Qian, X. Chen and Q. Chen, *Electrophoresis*, 2017, DOI: 10.1002/elps.201600529, n/a-n/a.
45. Q. Wei, D. Wu, B. Du, Y. Li and C. Duan, *Spectrochim. Acta Part A*, 2006, **63**, 532-535.
46. Y. Yue, X. Chen, J. Qin and X. Yao, *J. Pharm. Biomed. Anal.*, 2009, **49**, 753-759.
47. Y. L. Jiang, *Bioorg. Med. Chem.*, 2008, **16**, 6406-6414.
48. S. Bi, T. Zhao, Y. Wang and H. Zhou, *Luminescence*, 2016, **31**, 372-379.
49. S.-m. Song, X.-l. Hou, Y.-b. Wu, S.-m. Shuang, C. Yang, Y. Inoue and C. Dong, *J. Luminescence*, 2009, **129**, 169-175.

50. E. Alarcon, A. M. Edwards, A. Aspee, F. E. Moran, C. D. Borsarelli, E. A. Lissi, D. Gonzalez-Nilo, H. Poblete and J. C. Scaiano, *Photochem. Photobiol. Sci.*, 2010, **9**, 93-102.
51. S. Khan, B. Islam and A. Khan, *Int. J. Integ. Biol.*, 2007, **1**, 102-112.
52. S. N. Khan, B. Islam, R. Yennamalli, A. Sultan, N. Subbarao and A. U. Khan, *Eur. J. Pharm. Sci.*, 2008, **35**, 371-382.
53. N. Keswani and N. Kishore, *J. Chem. Therm.*, 2011, **43**, 1406-1413.
54. Z.-d. Qi, Y. Zhang, F.-l. Liao, Y.-w. Ou-Yang, Y. Liu and X. Yang, *J. Pharm. Biomed. Anal.*, 2008, **46**, 699-706.
55. H. Cheng, T. Zou, Y. Xu, Y. Wang, A. Wu, J. Dai, Y. Zhang and Y. Liu, *Luminescence*, 2016, **31**, 88-95.
56. A. Roy, D. Tripathy, A. Chatterjee and S. Dasgupta, *J. Biophys. Chem.*, 2010, **1**, 141-152.
57. D. Li, J. Zhu, J. Jin and X. Yao, *Journal of Molecular Structure*, 2007, **846**, 34-41.
58. Y. Yue, Y. Zhang, Y. Li, J. Zhu, J. Qin and X. Chen, *J. Luminescence*, 2008, **128**, 513-520.
59. J. He, Q. Wang, X. Ma, H. Yang, S. Li, K. Xu and H. Li, *J. Mol. Recog.*, 2016, **29**, 415-425.
60. S. Li, L. Wang, J. Hao, L. Wang, Y.-J. Tong, Z.-Q. Fu and A.-P. Zhang, *J. Appl. Spec.*, 2017, DOI: 10.1007/s10812-017-0410-x, 1-8.
61. Y.-Q. Wang, H.-M. Zhang and G.-C. Zhang, *J. Pharm. Biomed. Anal.*, 2006, **41**, 1041-1046.
62. P. Daneshgar, A. A. Moosavi-Movahedi, P. Norouzi, M. R. Ganjali, A. Madadkar-Sobhani and A. A. Saboury, *Int. J. Biol. Macromol.*, 2009, **45**, 129-134.
63. G. Zhang, Y. Wang, H. Zhang, S. Tang and W. Tao, *Pest. Biochem. Phys.*, 2007, **87**, 23-29.
64. A. Divsalar, M. J. Bagheri, A. A. Saboury, H. Mansoori-Torshizi and M. Amani, *J. Phys. Chem. B*, 2009, **113**, 14035-14042.
65. D. Bose, D. Sarkar and N. Chattopadhyay, *Photochem. Photobiol.*, 2010, **86**, 538-544.
66. D. V. Suresh, H. G. Mahesha, A. G. Rao and K. Srinivasan, *Biopolymers*, 2007, **86**, 265-275.
67. W. Y. He, H. J. Chen, F. L. Sheng and X. J. Yao, *Spectrochim. Acta. Part A*, 2009, **74**, 427-433.
68. F. Ding, W. Liu, X. Zhang, L. J. Wu, L. Zhang and Y. Sun, *Spectrochim. Acta. Part A*, 2010, **75**, 1088-1094.
69. J. Dai, T. Zou, L. Wang, Y. Zhang and Y. Liu, *Luminescence*, 2014, **29**, 1154-1161.
70. B. Hess, H. Bekker, H. Berendsen and J. Fraaije, *J. Comput. Chem.*, 1997, **18**, 1463-1472.
71. E. Alarcon, A. M. Edwards, A. Aspee, C. D. Borsarelli and E. A. Lissi, *Photochem. Photobiol. Sci.*, 2009, **8**, 933-943.
72. Q. Zhou, J. Xiang, Y. Tang, J. Liao, C. Yu, H. Zhang, L. Li, Y. Yang and G. Xu, *Coll. Surf. B*, 2008, **61**, 75-80.
73. J. Tian, J. Liu, W. He, Z. Hu, X. Yao and X. Chen, *Biomacromolecules*, 2004, **5**, 1956-1961.

74. W. He, Y. Li, J. Tian, H. Liu, Z. Hu and X. Chen, *J. Photochem. Photobiol. A: Chemistry*, 2005, **174**, 53-61.
75. J. Tang, N. Lian, X. He and G. Zhang, *J. Mol. Structure*, 2008, **889**, 408-414.
76. V. M. d. S. Fragoso and D. Silva, *AIP Conference Proceedings*, 2015, **1702**, 120003.
77. C. Wang, Q. H. Wu, C. R. Li, Z. Wang, J. J. Ma, X. H. Zang and N. X. Qin, *Anal. Sci.*, 2007, **23**, 429-433.
78. P. B. Kandagal, S. M. T. Shaikh, D. H. Manjunatha, J. Seetharamappa and B. S. Nagaralli, *J. Photochem. Photobiol. A: Chemistry*, 2007, **189**, 121-127.
79. B. Schwarzingler and H. Falk, *Monatshefte für Chemie / Chemical Monthly*, 2004, **135**, 1297-1304.
80. J. Wu, R. Wei, H. Wang, T. Li and W. Ren, *J. Biochem. Molecular Toxicol.*, 2013, **27**, 463-470.
81. H. Pu, H. Jiang, R. Chen and H. Wang, *Luminescence*, 2014, **29**, 471-479.
82. H. N. Hou, Z. D. Qi, Y. W. Ouyang, F. L. Liao, Y. Zhang and Y. Liu, *J. Pharm. Biomed. Anal.*, 2008, **47**, 134-139.
83. Q. Li, W.-y. Yang, L.-l. Qu, H.-Y. Qi, Y. Huang and Z. Zhang, *J. Spectroscopy*, 2014, **2014**, 7.
84. J. Tian, J. Liu, J. Xie, X. Yao, Z. Hu and X. Chen, *J. Photochem. Photobiol. B: Biology*, 2004, **74**, 39-45.