Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Identification and analysis of stereoselective drug interactions with low-density lipoprotein by high-performance affinity chromatography

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Tables S1 and S2 on the following pages summarize the best-fit parameters that were obtained for each binding model that was examined in this work for *R*- and *S*-propranolol with low density lipoprotein (LDL). The LDL in these studies was immobilized onto a silica support and placed within a column for use in high-performance affinity chromatography.

Table S1. Binding parameters obtained for *R*-propranolol[a]

Binding model	Temperature (°C)	m_{L1} (mol)	K_{a1} (M^{-1})	m_{L2} (mol)	K_{a2} (M^{-1})	nK_a (M^{-1})[b]
Single interaction, non-saturable	20	-	-	-	-	$3.5 (\pm 0.1) \times 10^{5}$
	27	-	-	-	-	$4.3 (\pm 0.2) \times 10^{5}$
	37	-	-	-	-	$2.1 (\pm 0.1) \times 10^{5}$
Single groups of saturable sites	20	$1.4 (\pm 0.4) \times 10^{-7}$	$5.3 (\pm 1.5) \times 10^{3}$	-	-	-
	27	$6.6 (\pm 1.5) \times 10^{-8}$	$1.6 (\pm 0.5) \times 10^{4}$	-	-	-
	37	$3.8 (\pm 0.7) \times 10^{-9}$	$1.2 (\pm 0.3) \times 10^{4}$	-	-	-
Two interactions, saturable + non-saturable[c]	20	**$9.0 (\pm 3.2) \times 10^{-10}$**	**$4.3 (\pm 3.4) \times 10^{5}$**	-	-	**$3.2 (\pm 0.1) \times 10^{5}$**
	27	**$3.0 (\pm 0.9) \times 10^{-9}$**	**$4.4 (\pm 2.7) \times 10^{5}$**	-	-	**$3.5 (\pm 0.2) \times 10^{5}$**
	37	**$7.5 (\pm 1.5) \times 10^{-10}$**	**$5.2 (\pm 2.3) \times 10^{5}$**	-	-	**$1.9 (\pm 0.1) \times 10^{5}$**
Two groups of saturable sites	20	$9.0 (\pm 9.7) \times 10^{-10}$	$4.3 (\pm 6.2) \times 10^{5}$	$1.3 (\pm 9490) \times 10^{-3}$	0.5 (± 3491)	-
	27	$3.0 (\pm 2.8) \times 10^{-9}$	$4.4 (\pm 5.2) \times 10^{5}$	$7.9 (\pm 87342) \times 10^{-4}$	0.8 (± 9313)	-
	37	$7.5 (\pm 5.7) \times 10^{-10}$	$5.2 (\pm 4.8) \times 10^{5}$	$7.0 (\pm 81917) \times 10^{-4}$	0.5 (± 5831)	-

[a]The numbers in parentheses represent a range of ± 1 S.D. All of these results were measured in the presence of pH 7.4, 0.067 M potassium phosphate buffer.

[b]The value for nK_a for a non-saturable interaction was obtained by dividing the best-fit result for $m_L K_a$ by the estimated moles of LDL. This latter value was obtained by using the protein content of the LDL support, a typical protein content for LDL of 25% (*w/w*), and an average molar mass for LDL of 2.3×10^6 g/mol [17].

[c]The results in bold are for the model that was determined to give the best description of the data.

Table S2. Binding parameters obtained for *S*-propranolol with LDL[a]

Binding model	Temperature (°C)	m_{L1} (mol)	K_{a1} (M^{-1})	m_{L2} (mol)	K_{a2} (M^{-1})	nK_a (M^{-1})[b]
Single interaction, non-saturable[c]	20	-	-	-	-	**$3.2 (\pm 0.1) \times 10^5$**
	27	-	-	-	-	**$2.8 (\pm 0.1) \times 10^5$**
	37	-	-	-	-	**$2.7 (\pm 0.2) \times 10^5$**
Single groups of saturable sites	20	$2.0 (\pm 1.8) \times 10^{-7}$	$3.2 (\pm 3.1) \times 10^3$	-	-	-
	27	$4.6 (\pm 4.5) \times 10^{-7}$	$1.2 (\pm 1.2) \times 10^3$	-	-	-
	37	$2.6 (\pm 2.4) \times 10^{-7}$	$2.0 (\pm 1.9) \times 10^3$	-	-	-
Two interactions, saturable + non-saturable	20	$0.1 (\pm 1.3) \times 10^{-5}$	$0.1 (\pm 2.0) \times 10^5$	-	-	$5.4 (\pm 1294) \times 10^4$
	27	$0.7 (\pm 6.0) \times 10^{-7}$	$0.6 (\pm 4.6) \times 10^5$	-	-	$2.7 (\pm 0.52) \times 10^5$
	37	$0.1 (\pm 1.6) \times 10^{-7}$	$0.2 (\pm 2.3) \times 10^5$	-	-	$2.2 (\pm 5.38) \times 10^4$
Two groups of saturable sites	20	$0.1 (+ 6.3) \times 10^{-5}$	$0.1 (+ 4.5) \times 10^5$	$2.0 (\pm 96665940) \times 10^{-4}$	0.2 (± 6848026)	-
	27	$4.9 (\pm 2636) \times 10^{-9}$	$0.1 (\pm 3.3) \times 10^6$	$8.2 (\pm 3776061) \times 10^{-4}$	0.6 (± 268838)	-
	37	$6.7 (\pm 2398) \times 10^{-9}$	$0.1 (\pm 2.4) \times 10^6$	$7.6 (\pm 4477418) \times 10^{-4}$	0.6 (± 318741)	-

[a]The numbers in parentheses represent a range of ± 1 S.D. All of these results were measured in the presence of pH 7.4, 0.067 M potassium phosphate buffer.

[b]The value for nK_a for a non-saturable interaction was obtained by dividing the best-fit result for $m_L K_a$ by the estimated moles of LDL. This latter value was obtained by using the measured protein content of the LDL support, a typical protein content for LDL of 25% (*w/w*), and an average molar mass for LDL of 2.3×10^6 g/mol [17].

[c]The results in bold are for the model that was determined to give the best description of the data.