Supplementary Material

Table 3.

Statistical parameters of CoMSIA models.

model #	*test compounds*	*residual*	*n*	r_{cv}^2 (s_{cv})	*C*	r^2 (*s*)
relative binding affinity						
1	*α-methyldigoxin* *digitoxigeninbisdigitoxoside* *proscillaridin A* *strophanthidol*	+ 0.20 + 0.22 + 0.11 + 0.01	33	0.42 (0.69)	3	0.79 (0.42)
2	*cymarin* *digitoxigenin* *gitoxin* *neriifolin*	+ 0.10 + 0.42 - 0.02 + 0.07	33	0.41 (0.70)	3	0.79 (0.41)
3	*16-acetylgitoxin* *peruvoside* *oleandrin* *gitoxigenin*	- 0.32 + 0.22 - 0.65 - 0.32	33	0.44 (0.68)	3	0.81 (0.39)
final	-	-	37	0.49 (0.64)	3	0.81 (0.39)
relative inhibitory potency						
1	*digitoxin* *digoxigeninbisdigitoxoside* *oleandrin* *ouabagenin*	+ 0.21 - 0.27 - 0.45 + 0.09	32	0.47 (0.36)	5	0.93 (0.14)
2	*anthroylouabain* *digitoxigeninmonodigitoxoside* *lanatoside C* *neriifolin*	+ 0.33 + 0.28 + 0.10 - 0.04	32	0.38 (0.38)	5	0.91 (0.14)
3	*cymarin* *digoxigenin* *proscillaridin A* *strophanthidin*	- 0.13 + 0.38 - 0.19 - 0.28	32	0.38 (0.38)	5	0.92 (0.13)
final	-	-	36	0.48 (0.34)	5	0.90 (0.15)

residual: observed minus predicted activity (logarithmic). r_{cv}^2: square of cross-validation correlation coefficient. s_{cv}: standard error of prediction. r^2: square of conventional correlation coefficient. *s*: standard error of estimate. *C*: number of components.