

Supplementary Materials

Table S1. Structures and negative inotropic activity data of the 29 compounds of the training set.

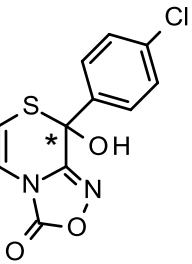
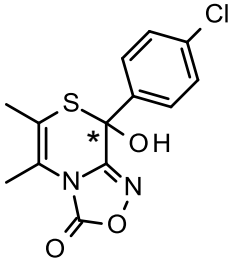
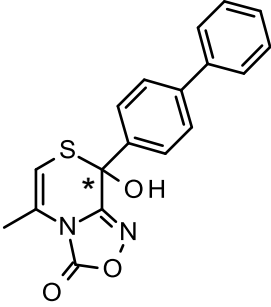
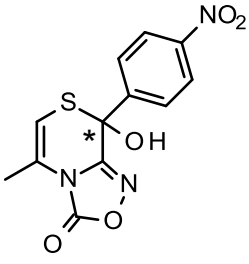
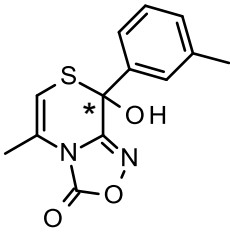
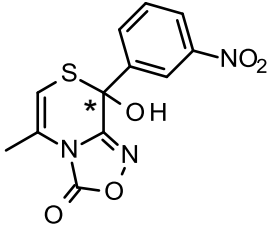
Source ^a	Molecule	Structure ^b	EC ₅₀ (μM)	pEC ₅₀
[1]	4b		4.07	5.390
[1]	4c		1.42	5.848
[1]	4i		2.65	5.577
[1]	4l		1.65	5.783
[1]	4n		0.65	6.187
[1]	4p		1.76	5.754

Table S1. *Cont.*

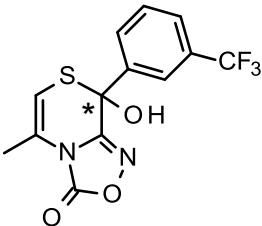
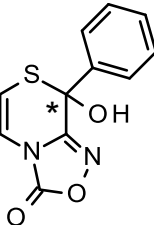
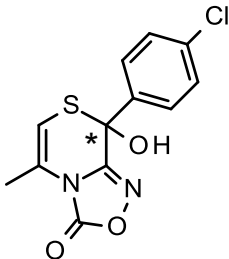
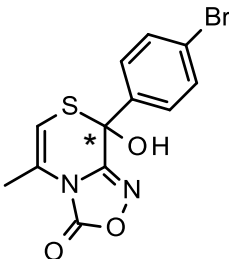
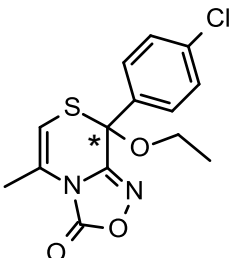
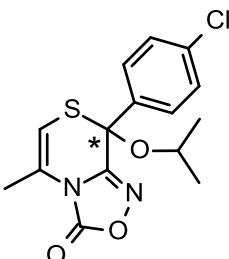
Source ^a	Molecule	Structure ^b	EC ₅₀ (μM)	pEC ₅₀
[1]	4q		2.17	5.664
[1]	6		6.58	5.182
[2]	1a		0.80	6.097
[2]	1b		0.32	6.495
[2]	5a		0.27	6.569
[2]	14a		0.22	6.658

Table S1. *Cont.*

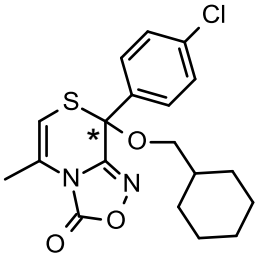
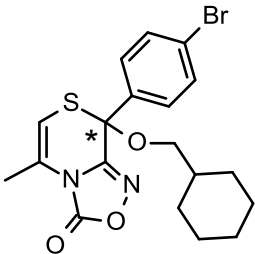
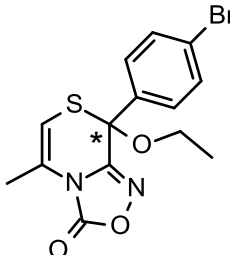
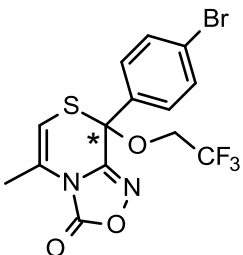
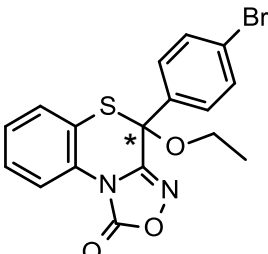
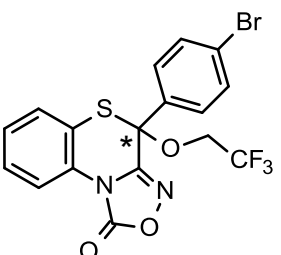
Source ^a	Molecule	Structure ^b	EC ₅₀ (μM)	pEC ₅₀
[2]	20a		0.24	6.620
[2]	20b		0.19	6.721
[2] Present paper	5b 25		0.04	7.398
[3] Present paper	2b 26		0.022	7.658
[3] Present paper	3a 28		0.013	7.886
[3] Present paper	3b 29		0.006	8.222

Table S1. *Cont.*

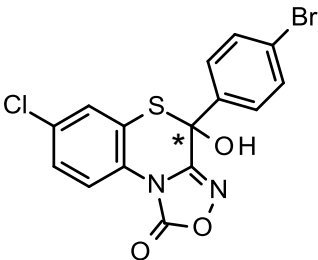
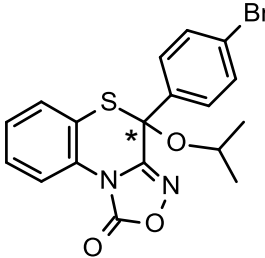
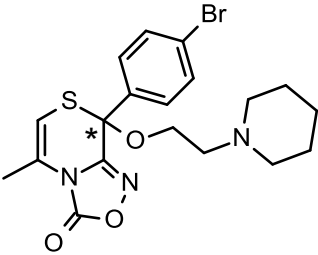
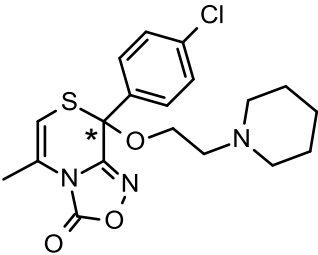
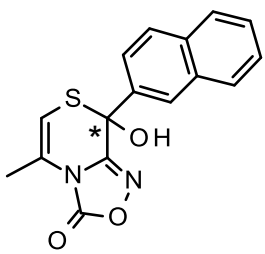
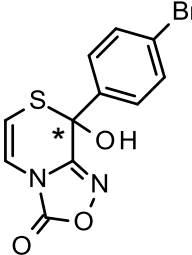
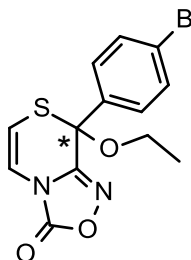
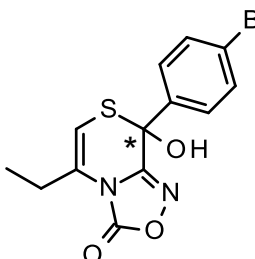
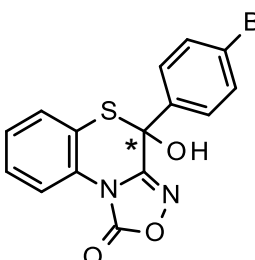
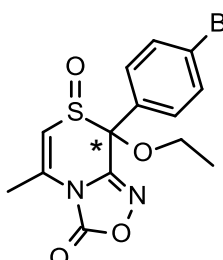
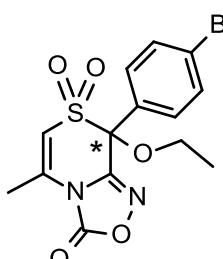
Source ^a	Molecule	Structure ^b	EC ₅₀ (μM)	pEC ₅₀
Present paper	30		0.36	6.444
Present paper	31		0.44	6.357
Present paper	32		3.67	5.435
Present paper	33		5.25	5.280
Present paper	34		0.057	7.244
Present paper	35		0.13	6.886

Table S1. Cont.

Source ^a	Molecule	Structure ^b	EC ₅₀ (μM)	pEC ₅₀
Present paper	36		0.039	7.409
Present paper	37		1.11	5.955
Present paper	38		4.23	5.374
Present paper	39		1.08	5.967
Present paper	40		0.76	6.119

^a References are listed below. ^b Although the data refer to the racemic mixture of the compounds, we used in the modeling the *R*-form.

References

1. Budriesi, R.; Cosimelli, B.; Ioan, P.; Lanza, C.Z.; Spinelli, D.; Chiarini, A. Cardiovascular characterization of [1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one-derivatives: Selective myocardial calcium channel modulators. *J. Med. Chem.* **2002**, *45*, 3475–3481.
2. Budriesi, R.; Carosati, E.; Chiarini, A.; Cosimelli, B.; Cruciani, G.; Ioan, P.; Spinelli, D.; Spisani, R. A New Class of Selective Myocardial Calcium Channel Modulators. 2. The Role of the Acetal Chain in Oxadiazol-3-one Derivatives. *J. Med. Chem.* **2005**, *48*, 2445–2456.
3. Carosati, E.; Ioan, P.; Barrano, G.B.; Caccamese, S.; Cosimelli, B.; Devlin, F.J.; Severi, E.; Spinelli, D.; Superchi, S.; Budriesi, R. Synthesis and Absolute Configuration Determination of New Oxadiazolothiazinones Active as L-Type Calcium Channel Blockers. *Eur. J. Med. Chem.* **2014**, submitted.