

## Supporting Informations

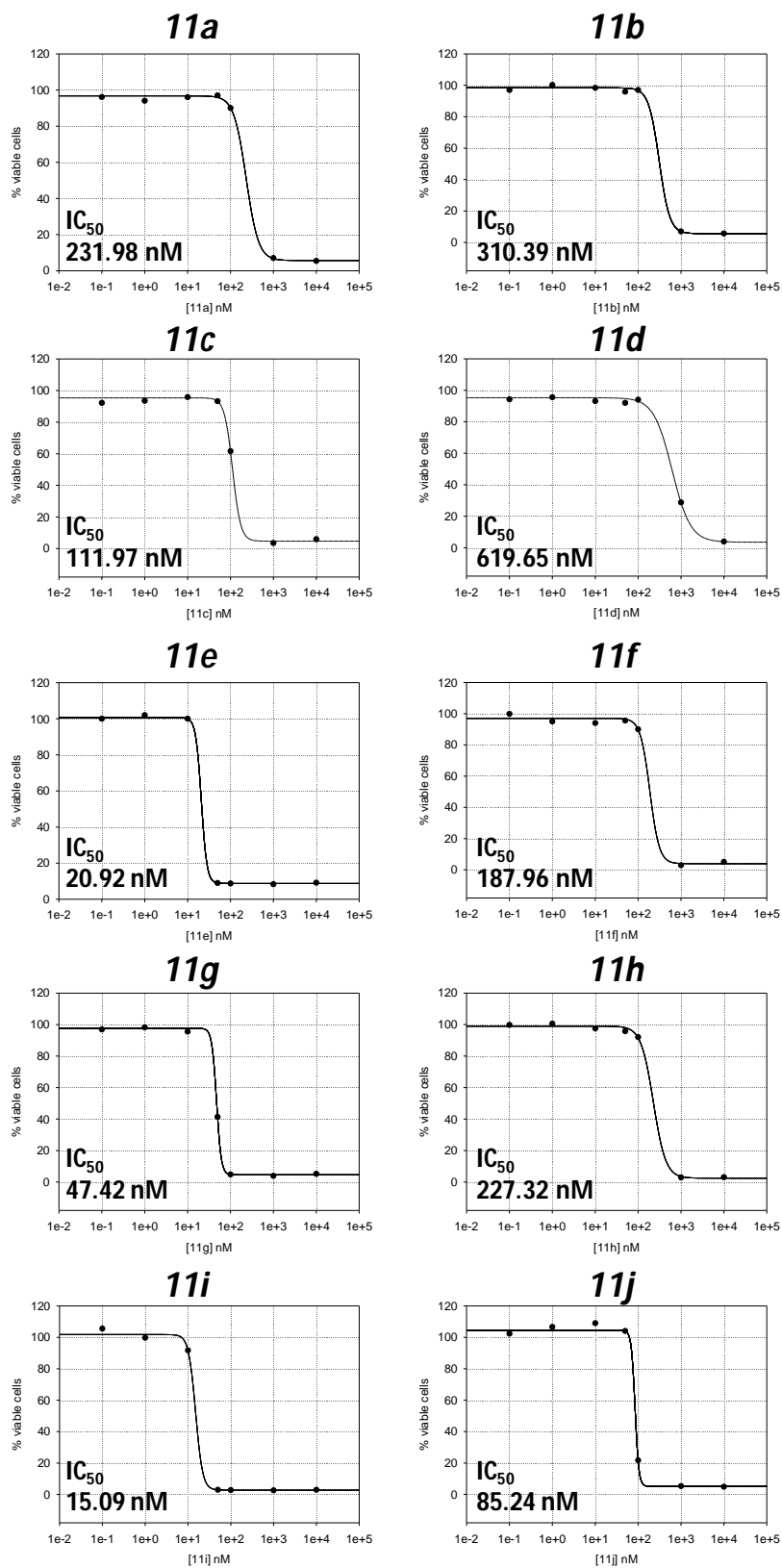
Compound ID (enantiomers RR)	Cluster population	E / kcal mol <sup>-1</sup>
11a	11	-4.44
11b	13	-4.39
	22	-2.64
11c	14	-4.64
11d	22	-3.84
11e	16	-4.99
	37	-4.42
11f	27	-3.71
11g	25	-4.57
11h	28	-5.37
11i	85	-5.16
11j	15	-5.7
	38	-5.5
2b	16	-4.11
	45	-4.02
	32	-3.97

**Table S1: Docking results for RR enantiomers. Only clusters with more than 10 conformations are reported.**

Compound ID (enantiomers SS)	Cluster population	E / kcal mol <sup>-1</sup>
11a	47	-5.56
	29	-3.88
11b	53	-5.74
11c	27	-5.85
	44	-4.17
11d	66	-4.01
11e	59	-5.22
11f	45	-3.76
11g	34	-4.61
11h	47	-6.34
11i	100	-5.61
11j	29	-5.46
	65	-5.16
2a	92	-5.02

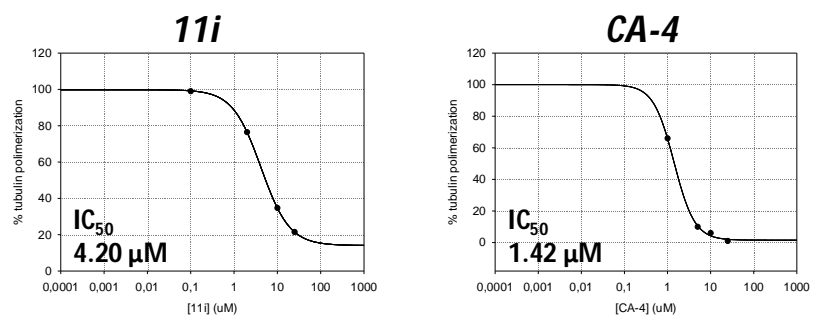
**Table S2: Docking results for SS enantiomers.**

## Supplementary Figure S1



**Figure S1.** Representative plots of inhibition vs concentration with fit-curves of compounds **11a-j**. Mean  $IC_{50}$  values are reported in Table 1.

## Supplementary Figure S2



**Figure S2.** Representative plots of tubulin polymerization inhibition with fit-curves of compounds **11i** and **CA-4**. Mean  $IC_{50}$  values are reported in Table 2.