

## Supplementary materials

**Table S1**

In silico-based aqueous solubility analysis of the marine aldehyde derivatives.

Marine aldehyde Derivatives	Log Sw	Level	Drug-likeness
MAD-1	-1.296	4	Optimal
MAD-2	-1.295	4	Optimal
MAD-3	-1.292	4	Optimal
MAD-4	-0.823	4	Optimal
MAD-5	-3.019	3	Good
MAD-6	-2.755	3	Good
MAD-7	-2.756	3	Good
MAD-8	-2.772	3	Good
MAD-9	-2.772	3	Good
MAD-10	-2.756	3	Good
MAD-11	-1.747	4	Optimal

Log Sw, the logarithm of the aqueous solubility

**Table S2**

Key to aqueous solubility levels indicator.

Level	Value	Drug-likeness
0	$\log(Sw) < -8.0$	Extremely low
1	$-8.0 < \log(Sw) < -6.0$	No, very low, but possible
2	$-6.0 < \log(Sw) < -4.1$	Yes, low
3	$-4.1 < \log(Sw) < -2.0$	Yes, good
4	$-2.0 < \log(Sw) < 0.0$	Yes, optimal
5	$0.0 < \log(Sw)$	No, too soluble
6	-1000	Warning: molecules with one or more unknown AlogP98 types

Log Sw, the logarithm of the aqueous solubility

**Table S3**

In silico-based BBB permeability analysis of the marine aldehyde derivatives.

Marine aldehyde Derivatives	Log BB	Level	Value
MAD-1	-0.341	2	Medium
MAD-2	-0.341	2	Medium
MAD-3	-0.341	2	Medium
MAD-4	-0.745	3	Low
MAD-5	0.006	1	High
MAD-6	-0.084	2	Medium
MAD-7	-0.084	2	Medium
MAD-8	-0.084	2	Medium
MAD-9	-0.084	2	Medium
MAD-10	-0.084	2	Medium
MAD-11	-0.514	2	Medium

Log BB, the logarithmic ratio between the concentration of a drug in the brain and blood

**Table S4**

Key to BBB permeability levels indicator.

Level	Value	Description
0	Very High	$\log \text{BB} \geq 0.7$
1	High	$0 \leq \log \text{BB} < 0.7$
2	Medium	$-0.52 < \log \text{BB} < 0$
3	Low	$\log \text{BB} \leq -0.52$
4	Undefined	Outside 99% confidence ellipse
5	AlogP98	Warning: molecules with one or more unknown AlogP98 types

Log BB, the logarithmic ratio between the concentration of a drug in the brain and blood