Discover natural compounds as potential phosphodiesterase-4B inhibitors via computational approaches

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Table S1
25 known PDE4B inhibitors from PDB

PDB ID	Ligand	IC ₅₀ (nM)
2QYL	NPV	650
1XLX	CIO	25
1XOT	VDN	3800
4MYQ	19T	32
3HNV	HBT	50.12
3WD9	QPC	8.3
3GWT	066	0.00794
3W5E	NVW	11
1XMU	ROF	0.84
1XOS	VIA	20000
1XLZ	FIL	960
3FRG	SK4	3.98
3D3P	20A	3.16
1XM6	5RM	420
1XMY	ROL	570
1R06	S, ROL	20~4000
1R06	R, ROL	20~4000
1XM4	PIL	0.041
1XN0	R, ROL	570
3G45	988	4.4
1XN0	S, ROL	570
1Y2J	7DE	33
4KP6	1S1	140
3LY2	Z72	5
1Y2H	6DE	56

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Table S2

Virtual screening results of DOCK and AutoDock Vina

Note: Thirty one molecules with pink backgroud are found in both hit groups.

	from DOCK		from Vina
ZINC67912533	-49.206142	ZINC03780340	-12.7
ZINC67912526	-45.246838	ZINC59779788	-12.3
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Discover natural compounds as potential phosphodiesterase-4B inhibitors via computational approaches

Journal of Molecular Modeling

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Table S3

Molecules that exist in both virtual screening results from DOCK and AutoDock Vina

Note: Four candidate PDE4B inhibitors are shown with pink background.

	DOCK score		Vina score
ZINC67912533	-49.206142	ZINC67912780	-12.1
ZINC67912770	-42.19717	ZINC67912765	-11.9
ZINC67912536	-41.430302	ZINC67912770	-11.6
ZINC67912780	-38.276733	ZINC67912773	-11.4
ZINC67912532	-37.361996	ZINC49823152	-11.2
ZINC72320416	-36.851089	ZINC28882432	-11.2
ZINC67912525	-36.755745	ZINC67902892	-11.1
ZINC72320169	-35.085491	ZINC08234294	-11
ZINC28882432	-33.335148	ZINC77269187	-10.8
ZINC03643476	-33.30909	ZINC72320169	-10.7
ZINC67913598	-33.271706	ZINC03872147	-10.6
ZINC67903429	-33.175091	ZINC67913598	-10.6
ZINC72320427	-32.940586	ZINC72320416	-10.5
ZINC67902910	-32.389038	ZINC67912525	-10.5
ZINC67912773	-31.671356	ZINC72320427	-10.4
ZINC77269187	-31.382269	ZINC67912532	-10.4
ZINC67902486	-31.349148	ZINC17654711	-10.4
ZINC67912765	-31.289375	ZINC67902910	-10.3
ZINC67902892	-31.123919	ZINC03643476	-10.3
ZINC67912413	-30.677685	ZINC31157937	-10.3
ZINC31157937	-30.339424	ZINC67912413	-10.3
ZINC03872147	-30.256912	ZINC31156607	-10.3
ZINC08234294	-30.152416	ZINC67903429	-10.2
ZINC67910582	-30.06736	ZINC77269545	-10.2
ZINC77269545	-29.98325	ZINC67912533	-10.2

ZINC31156607	-29.604549	ZINC67912536	-10.2
ZINC17654711	-29.54143	ZINC49601730	-10.2
ZINC67912484	-29.477083	ZINC67911752	-10.2
ZINC49601730	-29.394999	ZINC67910582	-10.1
ZINC67911752	-29.249697	ZINC67912484	-10.1
ZINC49823152	-29.1733	ZINC67902486	-10.1