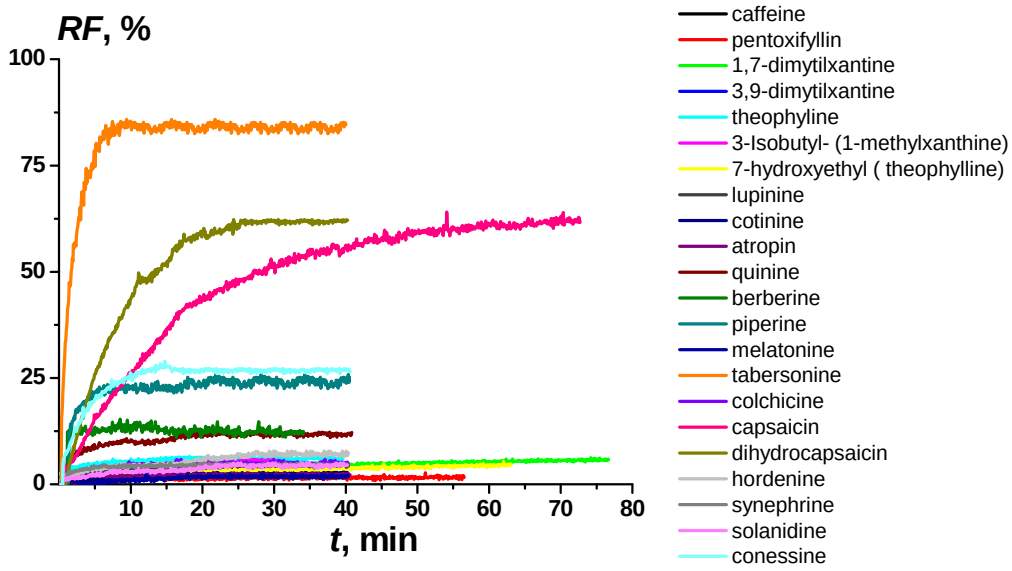
Supplementary Material

1.1 Supplementary Figures



Supplementary Figure 1. The time dependence of relative fluorescence of calcein (*RF*,%) leaked from POPC vesicles. Alkaloids were added into the liposomal suspension up to a concentration of 0.4 mM at the first time point. The relationship between the color line and the compound is given in the figure.

1.2 Supplementary Tables

Supplementary TABLE 1S. The physicochemical properties of tested alkaloids: *pKa* – the logarithm of acid dissociation constant, $LogD_{o/w}$ – the logarithm of octanol/water distribution coefficient at pH 7.4, $LogP_{o/w}$ – the logarithm of octanol/water partition coefficient, μ – molecule dipole moment.

Alkaloid	***pKa****		**$LogD_{o/w}$***	**$LogP_{o/w}$[#]**	**Reference**	**μ[$], D**	**μ[#], D**	**Reference**
	acidic	***basic***						
caffeine		-0.92	-0.55	-0.07, -0.08	Gaspari and Bonati, 1987; Lombardo et al., 2001; Kupsakova et al., 2004; Machatha and Yalkowsky, 2005; Schonsee and Bucheli, 2020	3.29	4.58, 4.23	Aaron and Gaye, 1987; Fischer et al., 1999
pentoxifylline	19.64	-0.93	0.23	0.29, 0.12	Lombardo et al., 2001; Hollosy et al., 2006	5.44	4.78	Augusto and Quintanilla, 2010
1,7-dimethylxanthine	10.76	-0.87	0.24	-0.24	Gaspari and Bonati, 1987	3.59	*na*	–
3,9-dimethylxanthine	8.99	1.09	-0.82	*na*		7.29	*na*	–
theophylline	7.82	-0.78	-0.89	-0.04, -0.02	Gaspari and Bonati, 1987; Kupsakova et al., 2004; Machatha and Yalkowsky, 2005	6.53	4.64, 7.66	Aaron and Gaye, 1987
3-isobutyl-1-methylxanthine	11.41	2.42	0.40	1.46[&]	Kupsakova et al., 2004	6.99	*na*	–
7-(β-hydroxyethyl) theophylline	15.43	-1.25	-1.24	*na*	–	2.26	*na*	–
lupinine	15.42	9.88	-1.52	*na*	–	1.24	*na*	–
cotinine		4.79	0.21	0.07	Li et al., 1992	4.95	*na*	–
atropine	15.15	9.39	-0.41	-0.55, 1.32, 1.82	Lombardo et al., 2001; Kuo et al., 2004; Machatha and Yalkowsky, 2005	3.58	4.39	Kuo et al., 2004

quinine	13.89	9.05	0.86	2.36, 2.79	Machatha and Yalkowsky, 2005; Hollosy et al., 2006	2.39	2.17	Karle and Bhattacharjee, 1999
berberine		*na*	-1.28	-1.03, -1.5	Schonsee and Bucheli, 2020; Wang et al., 2012	*na*	*na*	–
piperine		-0.13	2.78	2.25	Wu et al., 2012	5.37	5.98, 6.36	Gokalp, 2016
melatonin	15.8	-1.60	1.15	1.39, 1.2	Yu et al., 2016; Kanikkannan et al., 2001	4.93	4.76, 6.29	Zavodnik et al., 2006; Galijasevic and Hodzic, 2012
tabersonine	14.07	9.08	0.90	*na*	–	1.28	*na*	–
colchicine	15.06	-0.04	1.46	1.14, 1.2	Schonsee and Bucheli, 2020; Hollosy et al., 2006	6.53	*na*	–
capsaicin	9.93	-0.52	3.75	3.8	Hanson et al., 2015	4.66	3.96	Pereira et al., 2019
dihydrocapsaicin	9.93	-0.52	4.11	*na*	–	4.95	*na*	–
hordenine	10.31	9.19	0.06	*na*	–	0.99	1.49	Dwivedi et al., 2014
synephrine	9.76	9.15	-1.39	-0.45	Hansch and Zhang, 1995	2.32	2.82[@]	Cabezas et al., 2013
solanidine	18.2	12.47	1.39	*na*	–	1.24	*na*	–
conessine		10.53	-1.45	*na*	–	1.81	*na*	–

*The values of pKa and $LogD_{o/w}$ were predicted by ChemAxon

[$]Calculations of the dipole moments of the alkaloid molecules were performed by HyperChem 7.0 (Hypercube, Inc., Gainesville, FL, USA) using the semi-empirical MNDO

[#]Available literature data

[&]Partition coefficient of 1-isobutyl-3-methylxanthine

[@]Mean dipole moment of low-energy conformers

na = Not available

1.3 Supplementary References

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