

CAT'S CLAW OXINDOLE ALKALOID ISOMERIZATION INDUCED BY COMMON EXTRACTION METHODS

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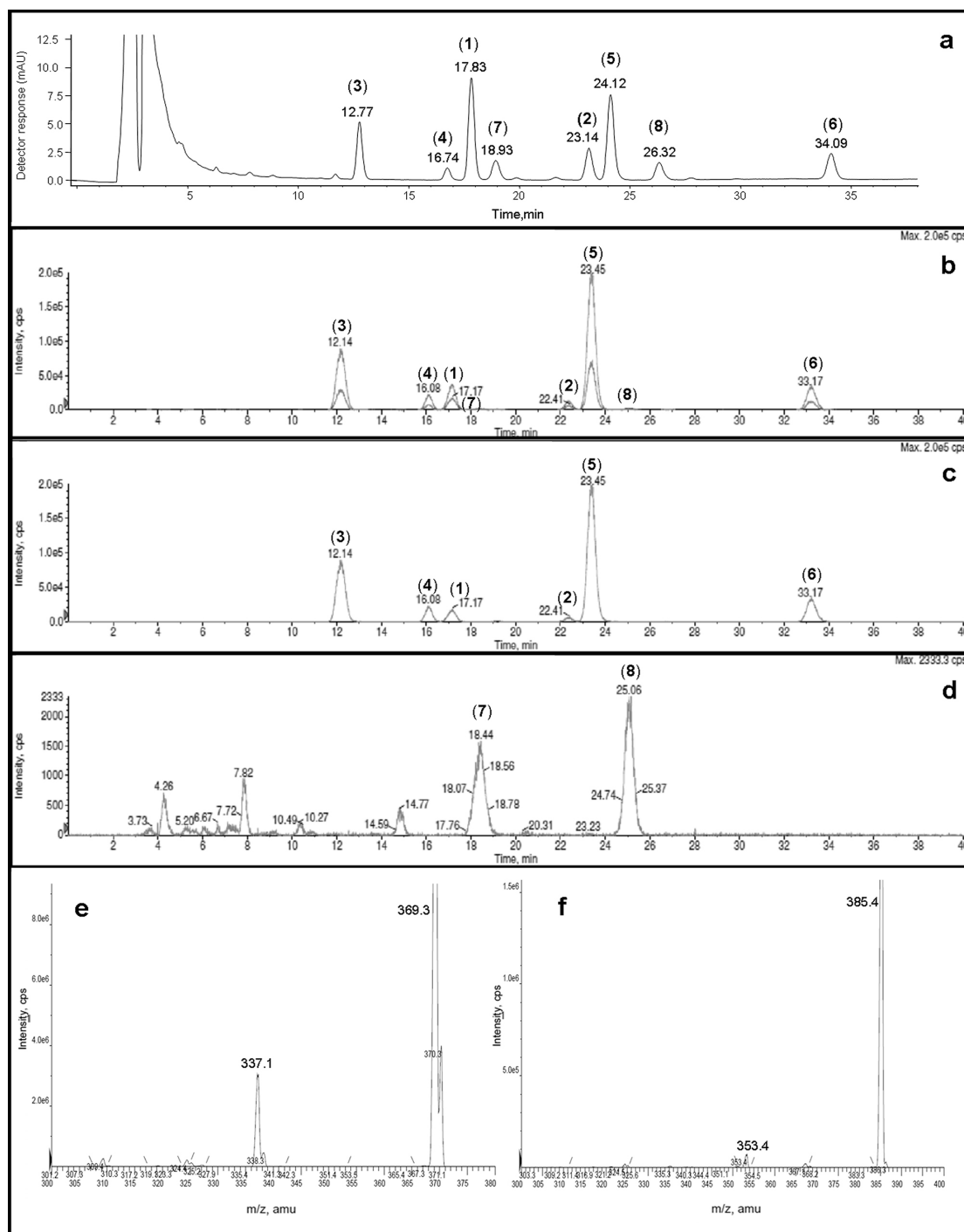


Figure 1S. HPLC-PDA profile of oxindole alkaloids in DM extract, at 245 nm (a); HPLC-MS/MS profiles monitoring the pseudomolecular ions $[M+H]^+$ at m/z 369.3 for pentacyclic oxindole alkaloid (POA), and m/z 385.4 for tetracyclic oxindole alkaloids (TOA) (b); Distinctive transitions of POA at m/z 369.3 \rightarrow 337.1 (c), and TOA at m/z 385.4 \rightarrow 353.4 (d); MS/MS spectra of POA (e), and TOA (f). Mitraphylline (1), isomitraphylline (2), speciophylline (3), uncarine F (4), pteropodine (5), isopteropodine (6), rhyncophylline (7), and isorhyncophylline (8)

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Table 1S. HPLC-PDA validation parameters concerning to individual alkaloid contents in dynamic maceration (DM) extract of cat's claw bark

Parameters	Pentacyclic oxindole alkaloid (POA)					Tetracyclic oxindole alkaloids (TOA)		
	mitraphylline (1)	isomitraphylline (2)	speciophylline (3)	uncarine F (4)	pteropodine (5)	isopteropodine (6)	rhynchophylline (7)	isorhynchophylline (8)
Peak purity index								
Extractive solution	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999
Reference compound	0.9999	0.9999	–	–	0.9999	0.9999	–	–
R²								
Extractive solution	0.9994	0.9988	0.9989	0.9984	0.9993	0.9987	0.9989	0.9988
Reference compound	0.9995	0.9994	–	–	–	–	–	–
Regression equation								
Extractive solution	y=55784x-658	y=20675x-1336	y=31011x+1835	y=5475.2x-658	y=53253x-3785	y=20802x-5131	y=13333x-917	y=12412x-1566
Reference compound	y=35492x-745	y=33708x-1766	–	–	–	–	–	–
LOD (µg/mL); LOQ (µg/mL)								
Reference compound	0.08; 0.24	0.09; 0.27	–	–	–	–	–	–
Repeatability (RSD %)								
Extractive solution	0.15	0.94	0.51	1.53	0.58	1.01	2.96	0.93
Reference compound	0.70	0.20	–	–	–	–	–	–
Intermediate precision (RSD %)								
Extractive solution	1.13	4.48	0.89	2.80	0.97	1.40	3.28	1.82
Reference compound	2.40	0.70	–	–	–	–	–	–
Recovery % ($\bar{X} \pm SD$)								
Reference compound	101.0 ± 0.5	101.9 ± 1.8	–	–	–	–	–	–

Coefficient of determination (R²); Limit of detection (LOD) and quantification (LOQ); Relative standard deviation (RSD%); mean ± standard deviation ($\bar{X} \pm SD$).

Table 2S. Coefficients of determination (R²) and regression variance (S) after fitting of kinetic data through linear and non-linear models

Alkaloid	Models: zero-order; first-order; second-order; Weibull; MMF	
	R ²	S
mitraphylline (1)	0.661; 0.717; 0.761; 0.999; 0.999	2.77; 0.05; 0.01; 0.16; 0.13
isomitraphylline (2)	0.650; 0.584; 0.516; 0.999; 0.999	2.30; 0.07; 0.01; 0.07; 0.17
speciophylline (3)	0.360; 0.435; 0.500; 0.999; 0.999	3.96; 0.18; 0.06; 0.05; 0.05
uncarine F (4)	0.730; 0.790; 0.823; ND; ND	0.28; 0.49; 0.05; ND; ND
pteropodine (5)	0.809; 0.798; 0.782; 0.999; 0.999	1.46; 0.02; 0.01; 0.04; 0.16
isopteropodine (6)	0.720; 0.569; 0.443; 0.999; 0.999	4.47; 0.13; 0.02; 0.32; 0.37
rhynchophylline (7)	0.589; 0.564; 0.537; 0.999; 0.999	4.54; 0.03; 0.01; 0.36; 0.23
isorhynchophylline (8)	0.589; 0.629; 0.658; 0.999; 0.999	4.54; 0.06; 0.01; 0.22; 0.23
Not determined (ND).		

Table 3S. Fitted values of the four-parameter Weibull model for kinetic curves of oxindole alkaloids on dynamic maceration (DM) extract after heating under reflux

Alkaloid	Parameter			
	a	b	c	d
mitraphylline (1)	29.68	19.78	2.84	-0.57
isomitraphylline (2)	21.45	11.29	0.13	0.92
speciophylline (3)	16.91	13.42	4.56	-1.81
pteropodine (5)	30.94	12.07	26.70	-1.06
isopteropodine (6)	37.14	29.35	0.24	0.57
rhynchophylline (7)	74.18	17.81	0.09	1.10
isorhynchophylline (8)	43.47	19.32	6.51	-1.15