The physicochemical properties and NMR spectra of some ergot alkaloids are summarized as following. Especially, under the influence of acids, alkaloids or light, the carbo at the position 8 of D-lysergic acid derivatives can occur isomerization which 8R is changed into 8S to form the responding isomers, lead to the formation of α-ergotaminine, ergocryptinine, ergocorninine and ergocristinine which the NMR data are shown in Table S1, S2 and S3.

Clavine

Agroclavine: crystal (acetone), mp 198~203℃, soluble in benzene, ethanol, slightly soluble in water. Molecular formula: $C_{16}H_{18}N_2$, MW *m/z*: 238. The data of ^{1}H-NMR (Pyridine-d_5，220 MHz) and ^{13}C-NMR (Pyridine-d_5，15.08 MHz) {Bach, 1974 #48}are shown in Table S1 and S2.

Elymoclavine: mp 250~252℃, Molecular formula: $C_{16}H_{18}N_2O$, MW *m/z*: 254. The data of ^{1}H-NMR ($CDCl_3$, 220 MHz) and ^{13}C-NMR ($CDCl_3$, 15.08 MHz){Bach, 1974 #48} of its acetate derivatives are shown in Table S1 and S2.

Festuclavine: mp 241℃, Molecular formula: $C_{16}H_{18}N_2$, MW *m/z*: 238. The data of ^{1}H-NMR ($CDCl_3$, 220 MHz) and ^{13}C-NMR ($CDCl_3$, 15.08 MHz) {Bach, 1974 #48}are shown in Table S1 and S2.

Fumigaclavine B: mp 265~267℃, Molecular formula: $C_{16}H_{20}N_2O$, MW *m/z*: 256. The data of ^{1}H-NMR (pyridine-d_5，220 MHz) and ^{13}C-NMR (pyridine-d_5，15.08 MHz) {Bach, 1974 #48}are shown in Table S1 and S2.

Ergoamides

Ergometrine: white crystal (acetone), mp 162℃. Molecular formula: $C_{19}H_{23}N_3O_2$, MW *m/z*: 325. ^{1}H-NMR (CD_3OD，500 MHz) δ: 1.11 (3H，d，J=6.0 Hz，C_{18}-CH_3), 2.53 (3H, s, N-CH_3) , 2.5 (1H, m, H-4β), 2.67 (1H, m, H-8) , 3.07-3.15 (2H, m, H-4α, 7β), 3.50 (4H, m, H-7α, 18, 19) , 3.95 (1H, m, H-5), 6.37 (1H, s, H-9) , 6.89 (1H, s, H-2), 7.00-7.13 (3H, H-12, 13, 14). The data of ^{13}C-NMR (DMSO, 15.08 MHz) {Bach, 1974 #48} are shown in Table S2.

Ergometrinine: white crystal (acetone), mp 195℃. Molecular formula: $C_{19}H_{23}N_3O_2$, MW *m/z*: 325. ^{1}H-NMR (pyridine-d_5) δ: 1.38 (3H, d, J=6.0 Hz, C_{18}-CH_3) , 2.45 (3H, s, N-CH_3), 2.61 (1H, q, J=4.1, 10.5 Hz, H-4β) , 2.91 (1H, m, H-8), 3.19 (2H, m, H-4α, 7β) , 3.30 (1H, m, H-18), 3.57 (1H, q, J=5.5, 11.0 Hz, H-7β), 3.77, 3.81 (1H, q, J=10.5Hz, H-19), 4.39 (1H, m, H-5) , 6.80 (1H, d, J=5.9 Hz, H-9), 7.11(1H, s, H-2), 7.25-7.40 (3H, m, H-12, 13, 14). The data of ^{13}C-NMR (DMSO, 15.08 MHz) {Bach, 1974 #48} are shown in Table S2.

Table S1 ^{1}H-NMR spectrum of clavines

	agroclavine		elymoclavine		elymoclavine acetate		festuclavine		fumigaclavine B	
	δ	J	δ	J	δ	J	δ	J	δ	J
4α	2.78	dd 15,12	2.89	dd 15,12	2.74	dd 15,12	2.68	dd 15,11.5	2.58	dd 11,11
4β	3.31	dd 15,4	3.37	dd 15,4	3.27	dd 15,4	3.39	dd 15,4.5	3.29	dd 11,2
5	2.52	ddd 12, 9.5,4	2.68	ddd 12, 9.5,4	2.53	ddd 12, 9.5,4	2.10	ddd 11.5, 9.5,4.5	2.66	ddd 11, 11,2
7α	3.24	d 17	3.65	d 17	3.37	d 17	2.95	d 11	3.38	d 12
7β	2.93	dd 17,4	3.08	dd 17,4	2.95	dd 17,4	1.87	t11	2.82	dd 12,4
8							2.01	ddd12, 11,6.5	2.15	m

9α 9β	6.18	s	6.80	s	6.47	s	2.63 1.08	dd12,3.5 q 12	4.51	s
10	3.74	dd 9.5,4	4.00	dd 9.5,4	3.76	dd 9.5,4	2.97	ddd 12, 9.5,3.5	2.58	d 11
17	1.77	s	4.45	s	4.66 4.46	d12	0.99	d 6.5	1.25	d 7
NMe	2.49	s	2.45	s	2.48	s	2.45	s	2.39	s

Table S2 ^{13}C-NMR spectrum of clavines, ergometrine and ergometrinine

	agroclavine	elymoclavine acetate	festuclavine	fumigaclavine B	ergometrine	ergometrinine
C-2	118.3	117.9	117.7	117.9	119.1	119.0
C-3	111.2	111.3	110.5	110.6	108.9	108.9
C-4	26.4	26.4	26.6	26.6	26.8	26.9
C-5	63.6	63.4	66.7	60.7	62.6	62.0
C-7	60.2	56.8	65.0	56.9	55.5	54.0
C-8	131.9	130.9	30.2	35.8	42.8	42.2
C-9	119.4	124.8	36.2	68.1	120.1	119.0
C-10	40.8	40.5	40.4	41.4	135.0	136.1
C-11	131.9	131.3	132.7	130.8	127.4	127.6
C-12	112.0	112.2	112.0	112.9	111.0	111.0
C-13	122.0	122.6	122.0	122.0	122.4	122.1
C-14	108.4	108.7	108.3	108.0	109.0	109.8
C-15	134.0	133.4	133.1	134.0	133.7	133.7
C-16	126.6	126.1	125.9	122.9	125.8	125.7
C-17	19.9	66.2	19.3	16.5	171.2	172.1
NMe	40.2	40.5	42.7	42.9	43.4	43.6
Me		20.6			17.4	17.2
C=O		170.7				
C-18					46.4	46.2
C-19					64.4	64.3

Ergopeptines

Ergotamine: mp 213~214℃, Molecular formula: $C_{33}H_{35}N_5O_5$, MW *m/z*: 581. The data of ^{13}C-NMR (DMSO, 15.08 MHz) {Bach, 1974 #48}are shown in Table S3.

Ergotaminine: mp 260℃, Molecular formula: $C_{33}H_{35}N_5O_5$, MW *m/z*: 581. The data of ^{13}C-NMR (DMSO, 15.08 MHz) {Bach, 1974 #48}are shown in Table S3.

α-ergocryptine: mp 212℃, Molecular formula: $C_{32}H_{41}N_5O_5$, MW *m/z*: 575. The data of ^{13}C-NMR ($CDCl_3$, 15.036 MHz) {Flieger, 1984 #50}are shown in Table S3.

β-ergocryptine: mp 173℃, Molecular formula: $C_{32}H_{41}N_5O_5$, MW *m/z*: 575. The data of ^{13}C-NMR ($CDCl_3$, 15.036 MHz) {Flieger, 1984 #50}are shown in Table S3.

α-Ergocryptinine: mp 240~242℃, Molecular formula: $C_{32}H_{41}N_5O_5$, MW *m/z*: 575. The data of ^{13}C-NMR ($CDCl_3$, 15.036 MHz) {Flieger, 1984 #50}are shown in Table S3.

Table S3 ^{13}C-NMR spectrum of ergopeptines

	ergotamine	ergotaminine	α-ergocryptine	β-ergocryptine	α-ergocryptinine
C-2	119.4	119.7	119.2	119.1	119.4
C-3	108.8	109.0	110.6	110.7	108.2
C-4	26.6	26.9	26.5	26.6	26.7
C-5	62.4	61.7	64.5	64.0	61.9
C-7	55.1	53.0	48.2	50.8	53.7
C-8	42.5	41.8	40.9	41.8	42.2
C-9	118.3	118.1	118.8	119.2	117.6
C-10	136.0	137.1	139.2	139.2	136.7
C-11	127.1	127.9	129.6	129.7	126.7
C-12	111.0	111.4	111.9	112.0	111.5
C-13	122.2	122.4	123.3	123.3	122.2
C-14	110.2	110.3	110.1	110.1	110.2
C-15	133.8	133.8	133.9	133.8	133.6
C-16	125.9	126.1	126.3	126.3	125.8
C-17	174.3	175.3	176.3	176.3	175.8
NMe	43.4	42.5	44.3	44.3	42.6
			Peptide part		
2′	85.9	85.7	89.7	89.5	89.1
3′	165.8	165.9	165.8	164.6	164.8
5′	56.1	56.1	53.3	59.7	52.3
6′	164.2	164.5	166.2	166.6	164.8
8′	45.8	45.7	46.0	45.9	45.5
9′	21.7	21.8	21.6	21.3	21.4
10′	25.9	25.9	22.2	22.2	25.9
11′	63.9	63.9	59.3	59.2	63.4
12′	102.8	102.9	103.4	103.6	102.8
13′	23.8	23.8	34.3	34.3	33.8
14′	38.7	38.7	15.3 [a]	15.3a	16.4 [a]
15′	138.7	138.9	16.9 [a]	17.0a	15.3 [a]
16′	129.9	129.9	43.5	39.4	42.6
17′	127.7	127.9	25.1	27.9	25.0
18′	127.4	126.1	22.1 [b]	12.6 [b]	22.2 [b]
19′	127.7	127.9	22.6 [b]	15.2 [b]	22.2 [b]
20′	129.9	129.9			

Note: [a b] value can be interchanged.

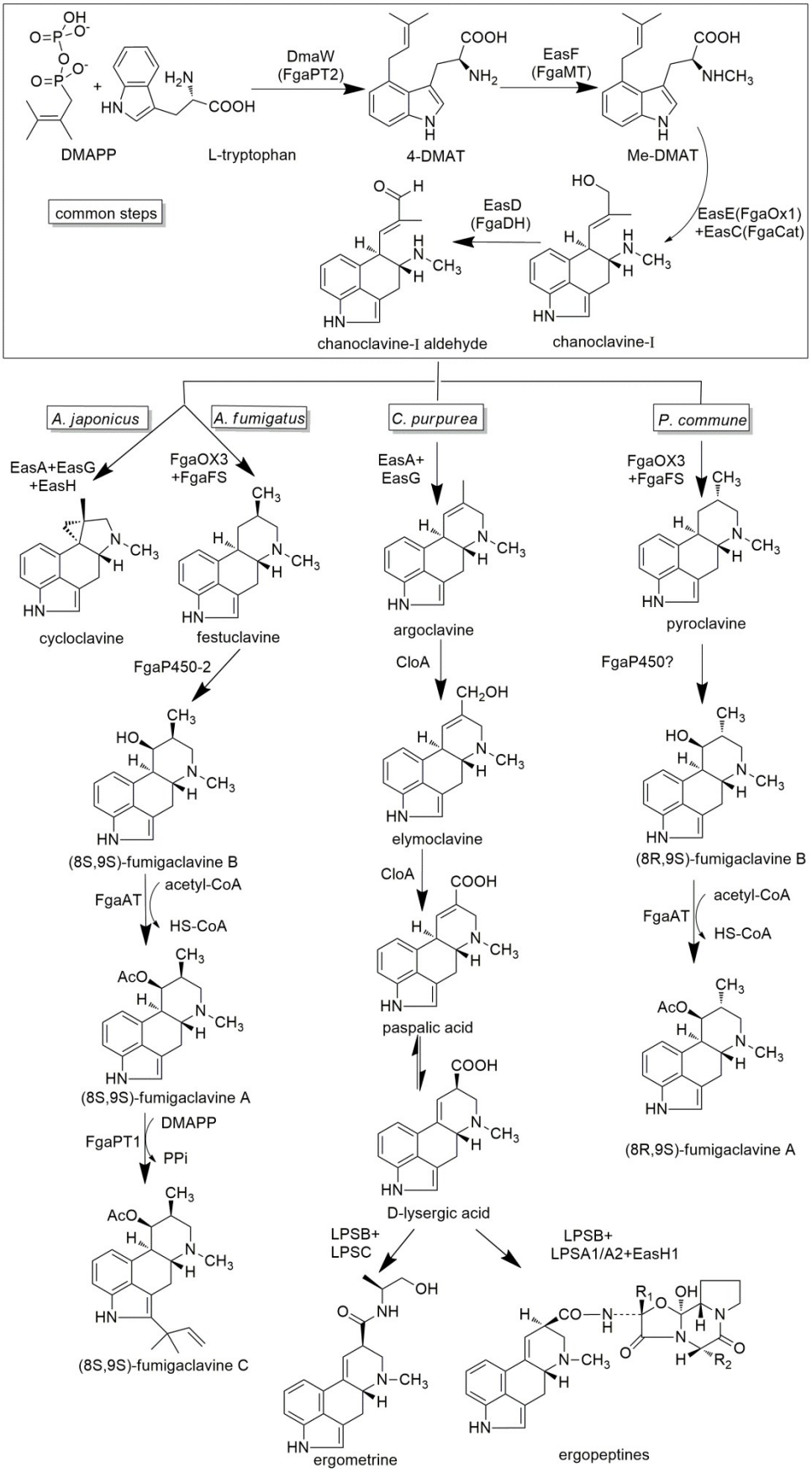

Fig. S1 The biosynthetic pathway of ergot alkaloids in different species (R1 and R2 represent different

group in the ergopeptines**)**