Supplementary File

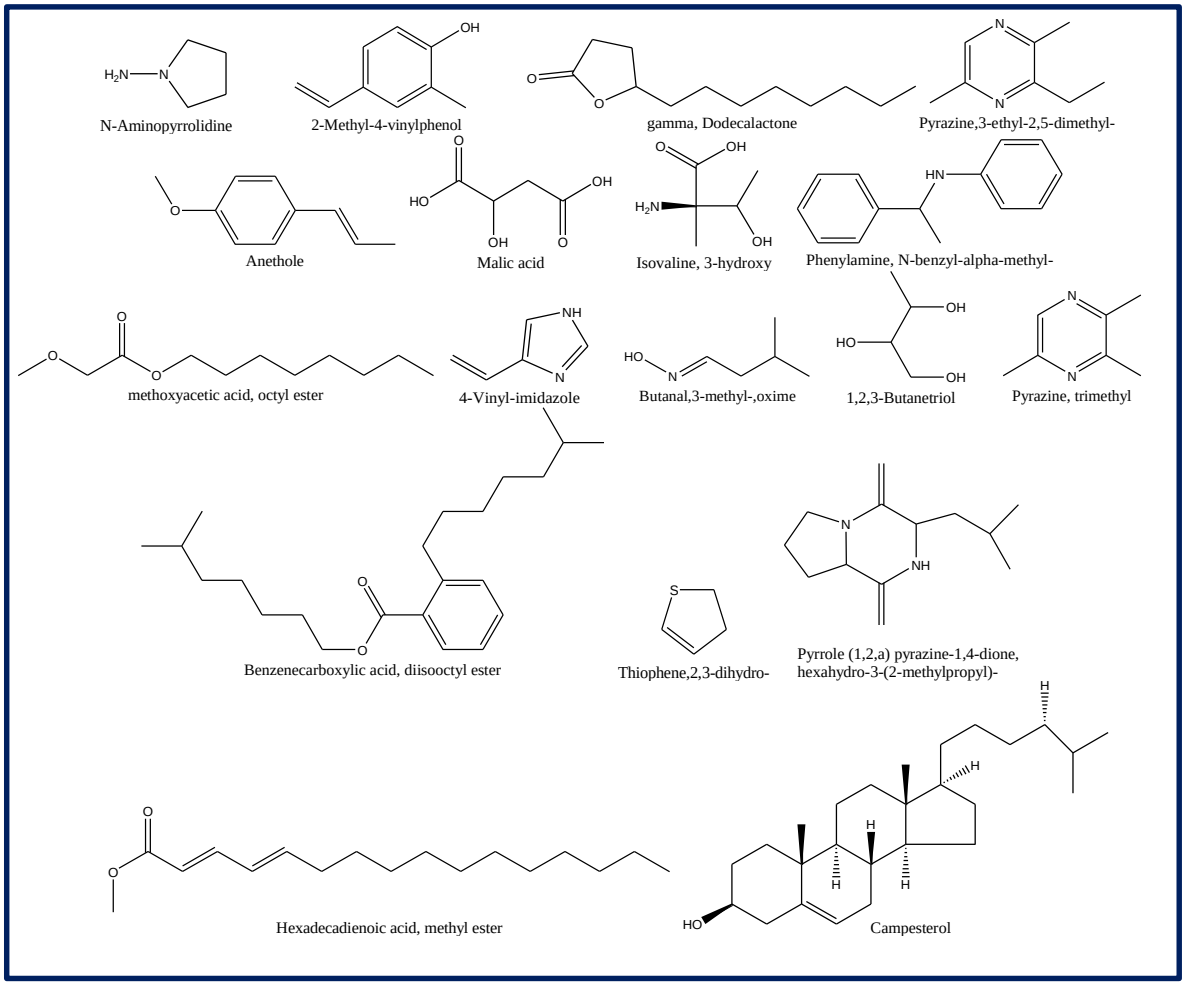

Figure S1. Structure of bioactive compounds present in lupin species.

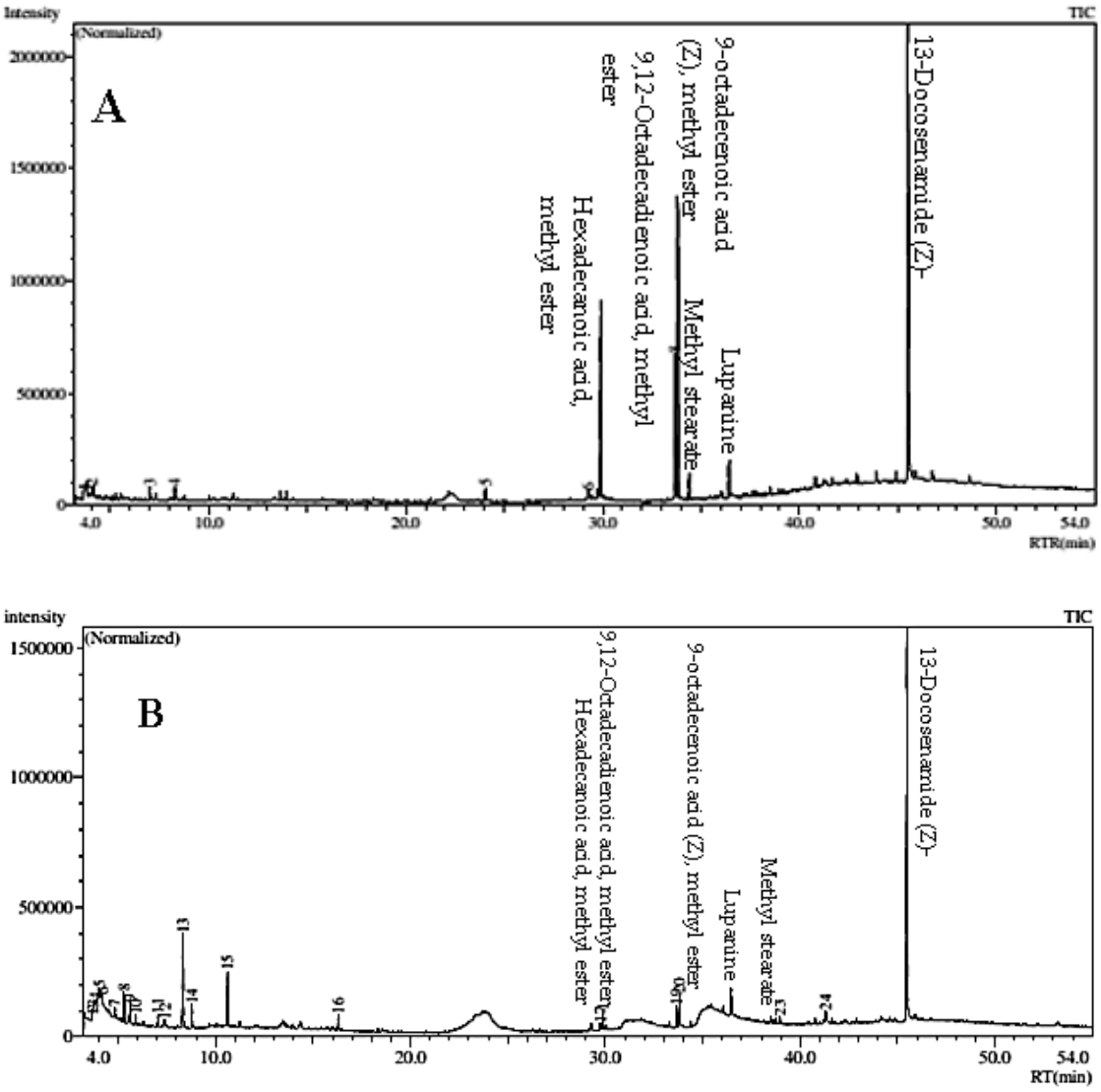

Figure S2. Common six compounds identified in unprocessed (A) and processed (B) flours of Lupin cultivar Jenabillup (JEN) in GC-MS analysis.

Table S1. Pharmacological activities of bioactive compounds present in lupin species.

Compound class	Bioactive compounds	Retention time (min)	m/z	Pharmacological activity	Ref
Quinolizidine alkaloid	Lupanine	36.44	136.00	Inhibition of lipid peroxidation and free radical scavenging, antidiabetic activities	[28,29]
	13-OH-Lupanine	41.29	152.00	Antioxidant activity	[31]
	13a-Acetoxylupanine	46.56	246.00	Antifungal, antibacterial activities	[34]
Fatty acid methyl ester	Hexadecanoic acid, methyl ester	33.64	67.00	Antifungal and antioxidant activities	[24]
	9,12-Octadecadienoic acid, methyl ester	33.64	67.00	Antioxidant and antimicrobial activities	[26]
	11-Octadecenoic acid, methyl ester	33.82	55.00	Antioxidant and antimicrobial activities	[26]
	Methyl sterate	34.40	74.00	Antioxidant activity	[27]
	7,10-Hexadecadienoic acid, methyl ester	38.68	67.00	Antioxidant, anti-inflammatory, hypocholesterolemic and cancer prevention activities	[30]
	9-Octadecenoic acid, methyl ester	33.83	55.00	Antioxidant activity	[26]
	Methyl tetradecanoate	24.05	74.00	Antifungal and antioxidant activities	[38]
	Dodecanoic acid, methyl ester	16.72	74.00	Antioxidant activity	[39]
	9-Hexadecenoic acid, methyl ester, (Z)-	33.80	55.00	Antioxidant activity	[26]
	1-Monolinoleoylglycerol Trimethylsilyl ether	38.52	73.00	Antioxidant, anticancer and antimicrobial activities	[48]
	Triacontanoic acid, methyl ester	41.67	149.00	Antioxidant activity	[49]
	Oleic acid, 3-hydroxypropyl ester	41.77	55.00	Antioxidant activity	[51]
	Methyl tetradecanoate	24.05	74.00	Antioxidant activity	[53]
	Methyl 9-cis,11-trans-octadecadienoate	34.73	67.00	Antioxidant activity	[54]
Volatile oil	Anethole	10.59	148.00	Antioxidant activity	[19]
Sterol	Campesterol	53.35	55.00	Antioxidant activity	[35]
Chromo-peptide	Actinomycin C2	29.49	154.00	Antimicrobial, antioxidant and anticancer activities	[23]
Amine	N-Aminopyrrolidine	8.42	85.00	Antioxidant activity	[17]
	13-Docosenamide, (Z)-	45.47	59.00	Antioxidant and antimicrobial activities	[33]
Heterocyclic compound	Pyrazine, 3-ethyl-2,5-dimethyl-	5.55	135.00	Antioxidant activity	[15]
	Pyrazine, trimethyl	4.186	122.00	Antioxidant activity	[15]
	Pyrazine, tetramethyl-	5.73	54.00	Antioxidant activity	[15]
	2-Pyrrolidione	5.94	85.00	Antioxidant activity	[17]
	Thiophene, 2,3-dihydro-	8.36	85.00	Antioxidant activity	[17]
	4-Vinyl-imidazole	8.53	94.00	Antioxidant activity	[18]
	pyrrole (1, 2, a) pyrazine 1, 4, dione, hexahydro 3-(2-methyl propyl)	29.77	70.00	Anticancer and anti-cholinesterase activities	[22]
	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-o	3.82	101.00	Antioxidant activity	[43]
	2-Piperidinone	5.68	85.00	Antioxidant activity	[44]
	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy	4.82	71.00	Antioxidant activity	[52]

Lactone	gamma, Dodecalactone	22.21	85.00	Antioxidant activity	[21]
Polyunsaturated hydrocarbon	Squalene	45.97	69.00	Antioxidant activity	[46]
Volatile compound	2,4-Decadienal, (E,E)-	11.42	81.00	Nematicidal Activity	[47]
Indole	(-)-Indole-2-one, 2,3-dihydro-3-[2-[N-dimeth	16.32	58.00	Antioxidant activity	[50]
Alcohol	1,2,3-Butanetriol	5.39	45.00	Antioxidant activity	[16]
	2-Methyl-4-vinylphenol	11.21	150.00	Antioxidant activity	[20]
	2-Methoxy-4-vinylphenol			Antioxidant activity	[45]
Carboxylic acid	Malic Acid	5.289	89.00	Antioxidant activity	[37]
Others	5,10-Diethoxy-2,3,7,8-tetrahydro-1H, 6H	30.00	70.00	Antioxidant activity	[25]
	1,2-Benzenecarboxylic acid, diisooctyl ester	41.67	149.00	Antioxidant activity	[32]
	Methoxyacetic acid, octyl ester	4.02	45.00	Antioxidant activity	[36]
	Divinyl sulfide	3.27	85.00	Antioxidant and antinociceptive activities	[42]
	Benzene, 1-methoxy-4-(1-propenyl)-	10.60	148.00	Antioxidant, anti-inflammatory and gastroprotector activities	[44]
	Butanal,3-methyl-,oxime	4.33	59.00	Antioxidant activity	[16]
	Di-n-octyl phthalate	41.67	149.00	Antioxidant activity	[55]

Table S2. Bioactive molecules obtained by GC-MS analysis in nine cultivars of processed and unprocessed lupin flours.

Compounds name	Concentration (%)																	
	BAR		GUN		JEN		JIN		MAN		LUX		ROS		WK		JUR	
	Un	P	Un	P	Un	P	Un	P	Un	P	Un	P	Un	P	Un	P	Un	P
Pyrazine, trimethyl				1.01		1.12	0.93			1.13		1.07						
Butanal,3-methyl-,oxime									12.30	8.97		23.04						
1-Propanol, 2-(2-hydroxypropoxy)-											0.19	0.99						
1,2,3-Butanetriol	2.44										1.43	2.24						
Pyrazine, 3-ethyl-2,5-dimethyl-									0.29			0.32						
Methoxyacetic acid, 2-methylpropyl ester									0.92			1.45		1.23				
Pyrazine, tetramethyl-											0.92	1.63						
2-Pyrrolidione							6.03	7.44				5.15		2.22		5.78		
Thiophene, 2,3-dihydro-						16.81	0.83	0.58	1.23	2.34		1.27	1.29					
N-Aminopyrrolidine											4.31	2.12	1.22					
4-Vinyl-imidazole												0.78	0.82	0.27				
Anethole				4.29		6.13		1.17	2.00			1.07				2.78		
2-Methyl-4-vinylphenol											1.92	1.18	3.09	2.18				
N-Hydroxymethyl-2-phenylacetamide									1.97			1.85						
Benzeneethanol, 4-hydroxy-			11.30								2.81	2.41						
Phenol, 2,4-bis(1,1-dimethylethyl)-									1.22	0.22		2.18						
Cyclohexane, pentyl-										1.23		1.32						
2(3H)-Furanone, dihydro-5-(2-octenyl)-, (Z)-							6.53	6.91	2.18			2.25						
Gamma, Dodecalactone							2.90	2.76	0.83		2.22	1.28						
3-Methyl-1,4-diazabicyclo(4.3.0)nonan-2,5-d										1.22	0.99	1.18						

Pyrrole (1, 2, a) pyrazine 1, 4, dione, hexahydro 3-(2-methyl propyl)				0.92	1.00	0.78	1.06	1.01	1.93			0.86						0.72
Actinomycin C2										0.68		2.33						
Hexadecanoic acid, methyl ester	31.06	5.73	8.52	6.28	25.92	2.87	2.29	1.32	18.30	2.89	18.22	2.67	0.23	0.11	10.08	3.29	2.91	20.70
5,10-Diethoxy-2,3,7,8-tetrahydro-1H, 6H												2.28						
Di(cyclopentanoyal-2)methane										1.55		0.5			1.46			
2-Pentylcyclopentanone												1.76						
9,12-Octadecadienoic acid, methyl ester	4.64	2.22	4.01	1.45	7.52	1.58	0.59	0.35	11.73	4.82	0.23	0.59	2.12	0.22	3.96	1.24	2.09	3.91
11-Octadecenoic acid, methyl ester	1.07	0.33	0.95	0.35	0.78	0.35	1.21	0.65	0.84	1.22	0.74	1.76	2.13	0.94	0.54	3.88	2.31	0.25
Phenylamine, N-benzyl-.alpha.-methyl-												0.38						
Methyl sterate	3.95	4.39	1.12	1.42	2.93	4.09	3.39	4.29	3.97	0.73	10.47	1.28	5.22	2.39	8.91	0.53	1.44	2.79
Lupanine	1.83	3.58	1.47	1.01	2.73	3.30	3.68	1.70	0.72	0.28	0.24	7.08	2.30	0.12	6.36	0.75	3.59	4.91
9-Octadecanamide									21.90			0.77						
7,14-Methano-4H,6H-dipyridol												0.21	0.11					
Ergotaman												1.05						
7,10-Hexadecadienoic acid, methyl ester									1.67			1.33	0.23					
9-Octadecenamide				0.54			0.36		1.06			0.45						
Ergotamine												0.88		0.21				
13-OH-Lupanine				0.64					1.21	0.81			0.19					
1,2-Benzenecarboxylic acid, diisooctyl ester												0.35						
13-Docosenamide, (Z)-	20.03	48.4	16.87	21.73	31.74	37.42	13.60	12.84	23.21	2.98	13.18	16.43	1.66	3.22	18.33	38.25	18.82	26.44

13a-Acetoxylupanine									9.22	1.88		0.32	0.11						
Campesterol				1.23								0.88							
Methoxyacetic acid, octyl ester										0.13									
Isovaline, 3-hydroxy	0.77								1.82										
Ethylene glycol monoisobutyl ether	3.01																		
Malic Acid	2.17			1.48		3.34	2.26	0.79				3.22			1.33		0.94		
9-Octadecenoic acid, methyl ester	11.44	3.34	7.54	5.99	14.09	2.18			15.64	0.09	0.28	5.31	2.34	23.87	0.55	2.19	12.68		
Nonanoic acid, 9-oxo-, methyl ester	0.58		0.37	0.32					0.39										
Benzeneethanol, 4-hydroxy-	12.32																		
Methyl tetradecanoate	3.49																		
Dodecanoic acid, methyl ester	1.06																		
9-Hexadecenoic acid, methyl ester, (Z)-	1.20			0.63					0.11		0.17	0.20							
1,2,3,4-Butanetetrol, [S-(R*,R*)]-		4.51																	
3,3-Dimethylbutane-2-ol		0.85										0.21	0.03						
dl-Mevalonic acid lactone		1.35							0.31										
cis-Methyl 11-eicosenoate			1.82																
Tetrapentacontane, 1,54-dibromo-			0.66							0.71		0.21							
13-Docosenoic acid, methyl ester, (Z)-			7.20	4.21					0.88		0.27	0.13	0.32						
Citronellol epoxide (R or S)			0.34							0.12		0.05							
2-Nonanol						7.09							0.23						
Divinyl sulfide						0.45													
dl-Glyceraldehyde						9.78													
2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-o						0.36													
Methoxyacetic acid, octyl ester						5.97													

2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl			1.90								0.42			0.60
Hexane-1,3,4-triol, 3,5-dimethyl-			2.31			1.82								
2-Amino-3-methyl-4-pentynoic acid			0.66											
N-Aminopyrrolidine			3.83											
1,4-Dioxane, 2,3-dimethoxy-				0.73							0.35			
1,3-Dioxolane, 2-methyl-				3.03		0.01								
2-Piperidinone				41.88	53.85									
4-Methylenebicyclo[4.2.0]oct-2-ene				1.36	1.30									
Phenol, 3,5-bis(1,1-dimethylethyl)-				1.04										0.41
L-Proline, N-valeryl-, heptadecyl ester	0.83			1.31		0.12								
Dodecanamide, N-isobutyl-				1.36	1.29									
N-Decanoylmorpholine				0.39	0.37					0.24				
4-Nitrobenzoylmethyl-.beta.-phenylpropionat				1.24	1.60									
N-Isobutyl-(6Z,8E)-decadienamide					0.25	0.11								
Hexanoic acid										2.99	0.12			0.81
dl-Malic disodium salt														0.30
Divinyl sulfide		2.02									0.21			0.93
Benzene, 1-methoxy-4-(1-propenyl)-														5.41
2-Methoxy-4-vinylphenol														0.46
1,2-Butanediol, 1-(2-furyl)-3-methyl-														0.47
Hydroxylupanine	0.31				0.64	0.02	0.99	0.13	0.72	0.08		0.09		0.18
Di-n-octyl phthalate														9.35
Squalene	1.05				0.12								1.17	0.93
Glycerin		4.81			28.09						20.10			
2,4-Decadienal, (E,E)-							0.63							
Nonanoic acid, 9-oxo-, methyl ester							1.44							

Cyclopropaneoctanoic acid, 2-[[2-[(2-ethylcy								0.24							
Eicosanoic acid, methyl ester	0.52					2.09		0.89							
Methyl 6-cis,9-cis,11-trans-octadecatrienoate							0.08	0.332							
1-Monolinoleoylglycerol trimethylsilyl ether								0.23							
Naphthalene, decahydro-1,5-dimethyl-								0.68							
Triacontanoic acid, methyl ester								0.17							
2-Hydroxy-gamma-butyrolactone							3.22					5.15			
13-Hydroxy-lupanine TMS derivative	0.22					0.03						0.60	0.56		
3-Allyloxy-1,2 propanediol													2.62		
1,3-Butanediol, 2-methyl-													3.38		
(-)-Indole-2-one, 2,3-dihydro-3-[2-[N-dimeth													3.66		
Pyridine, 1-acetyl-1,2,3,4-tetrahydro-5-(2-pip													0.30		
Di(cyclopentanonyl-2)methane													2.08		
Alpha-Isolupanine	0.74					18.31							15.45		
Oleic acid, 3-hydroxypropyl ester	0.72					1.01							3.65		
cis-13,16-Docasadienoic acid							0.91						1.89		
Methanone, dicyclopropyl-		3.58									0.15				
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy		1.34	1.39												
Methyl tetradecanoate		2.34									0.12				
1,4-Dioxane, 2,3-dimethoxy-				0.73	0.79					1.38					
Methyl 9-cis,11-trans-octadecadienoate				0.46	0.60										
N-Decanoylmorpholine				0.39	0.37		0.23								
Hexadecanoic acid, 2-hydroxy-1-(hydroxymet	0.21					1.03								1.03	0.40

Di-n-octyl phthalate	0.13	0.85	9.35

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