Relationship of glucosinolates thermal degradation and roasted rapeseed oil volatile odor

Xiaohui Mao, Xingzhong Zhao, Zongyao Huyao, Tingting Liu, Xiuzhu Yu*

Supplemental materials

Supplemental table captions:

Table S1 Iron contents in five rapeseeds.

Table S2 Parameters of accuracy and precision of GSLs determination method.

Table S3 GSLs Structures in rapeseed.

Table S4 Change of GSLs content in five rapeseeds during roasting.

Table S5Composition and content of volatile compounds in five RO during roasting.

Table S1 Iron contents in five rapeseeds

Samples	HZ	QH	DL	GS	SC
Content (mg/kg)	81.75±1.41c	121.77±4.19a	110.45±2.62b	128.10±3.78a	79.77±1.69c

Different superscript lettersndicate significant difference ($p < 0.05$).

Table S2. Parameters of accuracy and precision of GSLs determination method.

Recoveries of the internal standard (sinigrin)					
0.5μmol/g (n=6)		1μmol/g (n=6)		1.5μmol/g (n=6)	
Average[%]	RSD [%]	Average[%]	RSD [%]	Average[%]	RSD [%]
98.54	0.85	99.42	0.04	101.71	1.31

Table S3 GSLs Structures in five rapeseeds

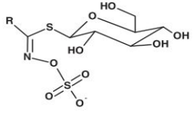
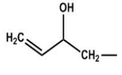
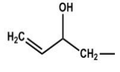
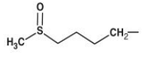
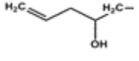
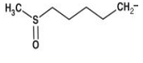
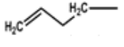
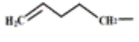
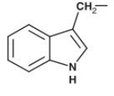
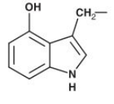
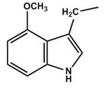
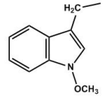
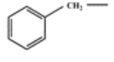
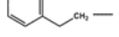
Basic structure of the GSLs													
													
GSLs group	Aliphatic							Indole				Aromatic	
Semisystematic name	2-Hydroxy-buten -3-yl	(E)-2-hydroxy-buten -3-yl	4-(Methylsulfiny l)butyl	2-Hydroxy 4-pentene	5-(Methylsulf inyl)pentyl	3-Butenyl	4-Pentene	3-Indolylmethy l	4-Hydroxy-3-in dolylmethyl	4-Methoxy -3- indole methyl	1-Methoxy -3- indole methyl	Benzyl	Phenethyl
Structural rest R													
Trivial name	Progoitrin	Epi-progoitrin	Glucoraphanin	Gluconapoleiferin	Glucoalyssin	Gluconapin	Glucobrassicanapin	Glucobrassicin	4-Hydroxygluco brassicin	4-Methoxygluc obrassicin	Glucobrassicin	Glucotropaeolin	Gluconasturtiin
Abbreviation	2-OH-3-But	E-2-OH-3-But	4-MSOB	2-OH-4-Pen	5-MSOP	3-BUT	4-Pen	IMG	4-OH-IMG	4-MeO-IMG	1-MeO-IMG	BEG	PEG

Table S4 Change of GSLs content in five rapeseeds during roasting

Samples	Concentration of GSLs (μmol/g)													
	Aliphatic							Indole				Aromatic		Total
	2-OH-3-But	E-2-OH-3-But	4-MSOB	2-OH-4-Pen	5-MSOP	3-BUT	4-Pen	IMG	4-OH-IMG	4-MeO-IMG	1-MeO-IMG	BEG	PEG	
HZ														
7-1	17.54±0.28a	—	1.22±0.05a	0.87±0.06a	0.19±0.00a	8.39±0.30a	2.04±0.03a	0.04±0.01b	5.36±0.22a	0.52±0.4b	0.02±0.00b	0.31±0.07a	0.22±0.04a	36.72±0.95a
7-2	16.30±0.31b	—	1.12±0.06b	0.80±0.06ab	0.16±0.03a	7.39±0.07b	1.94±0.07b	0.04±0.00b	5.54±0.07a	0.62±0.02a	0.02±0.00b	0.26±0.01ab	0.21±0.01a	34.41±0.48b
7-3	15.13±0.37c	—	1.06±0.01b	0.76±0.01b	0.14±0.04a	7.03±0.38b	1.79±0.02c	0.04±0.00b	5.26±0.05a	0.50±0.02b	0.03±0.00b	0.22±0.09b	0.23±0.02a	32.19±0.64c
7-4	14.61±0.44c	—	1.14±0.009b	0.81±0.01ab	0.15±0.06a	8.14±0.14a	1.83±0.03c	0.03±0.00b	4.88±0.29b	0.49±0.01b	0.03±0.01a	0.14±0.03c	0.13±0.03b	35.05±0.11c
7-5	14.56±0.05c	—	0.98±0.03c	0.73±0.04bc	0.18±0.08a	7.32±0.03b	1.87±0.00bc	0.05±0.00a	3.47±0.08c	0.40±0.01d	0.04±0.01a	0.13±0.00c	0.14±0.03b	29.87±0.18d
7-6	14.62±0.14c	—	1.08±0.03b	0.74±0.01bc	0.15±0.07a	7.33±0.13b	1.69±0.04d	0c	1.24±0.01d	0.28±0.01e	0c	0.14±0.01c	0.14±0.01b	27.37±0.29e
7-7	7.21±0.29d	—	0.71±0.03d	0.66±0.02c	0b	4.37±0.12c	0.96±0.03e	0c	0.08±0.01e	0.05±0.01f	0c	0.13±0.03c	0c	14.17±0.41f
SC														
7-1	21.39±0.14a	1.01±0.03a	1.05±0.03a	0.86±0.02a	0.14±0.02a	6.88±0.02a	2.39±0.06b	0.05±0.00a	6.51±0.27ab	0.48±0.04a	0.04±0.00a	0.35±0.01b	0.23±0.01b	41.38±0.40a
7-2	20.81±0.15b	1.05±0.21a	0.94±0.00c	0.75±0.03c	0.15±0.02a	6.40±0.02b	2.58±0.15a	0.05±0.03a	6.88±0.10a	0.46±0.04ab	0.03±0.00bcd	0.35±0.01b	0.18±0.02c	40.62±0.54a
7-3	20.65±0.37bc	1.05±0.13a	1.02±0.01ab	0.84±0.00a	0.15±0.00a	6.43±0.13b	2.34±0.00b	0.06±0.00a	6.71±0.13a	0.50±0.00a	0.04±0.00abc	0.40±0.00a	0.27±0.01a	40.47±0.25a
7-4	20.78±0.28b	1.00±0.13a	0.98±0.00bc	0.80±0.00b	0.15±0.00a	6.59±0.17b	1.92±0.04cd	0.05±0.01a	6.20±0.36b	0.47±0.04ab	0.03±0.01bcd	0.22±0.03d	0.27±0.02a	39.45±0.06b
7-5	20.20±0.16c	1.09±0.05a	1.04±0.03ab	0.85±0.03a	0.17±0.02a	6.92±0.22a	2.06±0.03c	0.05±0.00a	4.52±0.04c	0.41±0.00b	0.05±0.01a	0.24±0.01cd	0.20±0.01bc	37.78±0.35c
7-6	19.44±0.03d	0.79±0.21a	0.96±0.04c	0.73±0.01c	0.13±0.04a	6.66±0.04ab	1.83±0.09d	0b	1.44±0.07d	0.24±0.00c	0.02±0.00cd	0.26±0.01c	0.04±0.059d	32.54±0.42c
7-7	10.01±0.17e	0b	0.59±0.00d	0.55±0.01d	0b	3.96±0.06c	1.06±0.00e	0b	0.13±0.02e	0.06±0.01d	0.01±0.02d	0.11±0.01e	0e	16.48±0.28e
QH														
7-1	3.16±0.17a	—	0.84±0.05bc	0.24±0.02a	0.14±0.01b	35.90±0.11a	5.77±0.25a	0.03±0.01a	3.79±0.14a	0.20±0.01a	0.02±0.00a	0.17±0.00a	0.87±0.04a	51.13±0.07a
7-2	2.91±0.19ab	—	0.71±0.02de	0.22±0.01a	0.13±0.00b	30.62±0.26c	4.36±0.14bc	0.03±0.02a	3.04±0.01b	0.15±0.00b	0.02±0.00a	0.12±0.02b	0.50±0.01c	42.82±0.08c
7-3	2.63±0.25b	—	0.70±0.04e	0.26±0.02a	0.18±0.00a	33.56±0.66b	4.21±0.27c	0.04±0.00a	2.96±0.29b	0.15±0.02b	0.02±0.00a	0.10±0.01b	0.55±0.04c	45.35±1.56b

7-4	2.66±0.32b	—	0.94±0.06a	0.25±0.01a	0.17±0.01a	29.50±0.23d	4.90±0.13b	0.04±0.01a	2.78±0.56b	0.02±0.00c	0b	0.12±0.01b	0.58±0.01b	41.94±0.84c
7-5	2.10±0.00c	—	0.79±0.01cd	0.24±0.01a	0.11±0.00c	30.69±0.42c	4.80±0.54bc	0.03±0.00a	2.46±0.10b	0c	0b	0.12±0.01b	0.56±0.00b	41.91±0.86c
7-6	2.90±0.00ab	—	0.89±0.02ab	0.17±0.00b	0d	30.23±0.10cd	4.54±0.02bc	0b	0.86±0.01c	0c	0b	0c	0.38±0.02b	39.96±0.09d
7-7	1.04±0.02d	—	0.55±0.02f	0.12±0.02c	0d	18.74±0.46e	2.96±0.05d	0b	0.07±0.00d	0c	0b	0c	0d	23.47±0.49d
GS														
7-1	36.62±0.32a	4.59±0.56ab	1.01±0.08b	0.72±0.10abc	0.17±0.01a	15.31±0.04a	2.57±0.19ab	0.12±0.03a	6.53±0.3a	0.21±0.02b	0.04±0.02a	1.43±0.03a	0.31±0.01a	69.62±0.15a
7-2	36.36±0.54ab	4.83±0.18a	0.96±0.00b	0.79±0.02ab	0.16±0.01ab	15.59±0.18a	2.77±0.15a	0.13±0.01a	6.35±0.18a	0.18±0.03b	0.05±0.00a	1.32±0.00ab	0.30±0.06ab	69.79±1.17a
7-3	35.80±0.72ab	4.09±0.02abc	1.16±0.06a	0.82±0.03a	0.13±0.01ab	15.45±0.30a	2.76±0.01a	0.09±0.00a	6.10±0.13a	0.20±0.01b	0.05±0.00a	1.29±0.02b	0.24±0.01bc	68.20±0.78a
7-4	34.88±0.75bc	3.45±1.37abc	0.98±0.04b	0.79±0.04ab	0.15±0.04ab	13.89±0.37b	2.54±0.14ab	0.10±0.02a	6.06±0.05a	0.27±0.01a	0.05±0.00a	1.21±0.06bc	0.24±0.00c	64.61±0.05b
7-5	33.72±0.58c	2.97±0.79c	0.92±0.01bc	0.70±0.01bc	0.14±0.01ab	14.19±0.13b	2.55±0.16ab	0.10±0.02a	3.91±0.37b	0.18±0.00b	0.04±0.01a	1.13±0.08c	0.19±0.02c	60.73±0.61c
7-6	28.35±0.87d	2.52±0.81c	0.84±0.01c	0.63±0.02c	0.12±0.01b	12.12±0.41b	2.22±0.19b	0.05±0.01c	0.98±0.02c	0.09±0.02c	0.04±0.00a	0.71±0.09d	0.12±0.01d	48.80±0.82d
7-7	5.16±0.03d	0d	0.40±0.01d	0.24±0.03d	0.14±0.01ab	3.74±0.11b	0.79±0.13c	0d	0.10±0.03d	0d	0b	0.27±0.04e	0e	10.83±0.01e
DL														
7-1	56.19±0.06a	3.81±0.02ab	0.89±0.00a	2.06±0.01a	0.20±0.01a	25.43±0.06a	4.87±0.11a	0.09±0.00a	4.75±0.01a	0.14±0.05a	—	0.25±0.05a	0.33±0.01a	99.00±0.32a
7-2	54.15±1.02b	3.94±0.80a	0.72±0.04c	1.69±0.04c	0.20±0.00a	21.69±0.24c	4.47±0.11b	0.07±0.01b	3.79±0.09d	0.14±0.04a	—	0.27±0.02a	0.26±0.02a	91.36±0.71c
7-3	53.74±0.01b	3.40±0.18ab	0.89±0.04a	1.91±0.04b	0.19±0.01a	23.67±0.20b	4.26±0.16b	0.06±0.01b	4.49±0.14b	0.05±0.01b	—	0.16±0.00b	0.22±0.04b	93.04±0.02b
7-4	53.48±0.64b	3.93±0.14a	0.81±0.00b	1.89±0.04b	0.17±0.00ab	25.19±0.00a	4.37±0.32b	0.06±0.01b	4.15±0.18c	0.06±0.00b	—	0.18±0.01b	0.23±0.05b	94.51±0.40b
7-5	51.55±0.44c	3.03±0.16b	0.88±0.00a	2.02±0.01a	0.16±0.02bc	23.89±0.15b	3.67±0.12c	0.04±0.01c	2.87±0.08e	0.06±0.00b	—	0.17±0.04b	0.18±0.05b	88.52±0.83d
7-6	39.79±0.44d	3.70±0.37ab	0.66±0.01d	1.55±0.03d	0.12±0.01d	18.77±0.11d	3.65±0.09c	0d	0.94±0.05f	0.04±0.00b	—	0.17±0.01b	0.11±0.01b	69.49±0.37e
7-7	40.11±0.80d	3.12±0.05ab	0.73±0.03c	1.53±0.05d	0.14±0.01c	18.90±0.41d	3.75±0.06c	0d	0.37±0.03f	0.03±0.00b	—	0.15±0.01b	0c	68.83±1.24e

Note: "—", not detected; sample 7-1~7-7 represents RO which roasted for seven durations 0, 10, 20, 30, 40, 50 and 60 min, respectively.

Values with different letters in the same column of the same variety oil are significantly different ($p < 0.05$).

Table S5 Content and composition of volatile compounds in five RO during roasting

Compounds	Alkanes	Acids	Esters	Ketones	Aldehydes	Alcohols	Alkenes	Sulfur-containing compounds		Nitrogen-containing compounds			Oxygen heterocycle (furans and pyran)	Benzenes	Total
								Thiocyanates	Others	Nitriles	Pyrazines	Others			
HZ															
7-1	1.27±0.16a	0.09±0.01e	0.27±0.03e	0.66±0.08e	1.95±0.24e	3.56±0.43c	—	—	—	—	—	0.32±0.05d	—	0.10±0.14b	8.22±0.39e
7-2	0.12±0.02f	—	0.14±0.03f	0.54±0.10e	1.62±0.29e	2.10±0.36d	—	—	—	—	—	1.11±0.20b	—	0.60±0.11c	5.54±0.58f
7-3	0.40±0.07d	0.13±0.02e	0.36±0.06d	0.45±0.08f	1.33±0.24f	2.18±0.39d	—	—	—	—	—	0.79±0.14c	—	0.84±0.15b	5.64±0.68f
7-4	0.30±0.02e	0.51±0.03d	0.27±0.01e	0.93±0.05d	2.56±0.13d	1.76±0.09d	—	—	—	13.35±0.64d	—	1.11±0.05b	—	1.02±0.05b	20.80±0.71d
7-5	0.66±0.005c	2.32±0.02c	3.28±0.03b	1.84±0.02b	6.25±0.15c	2.24±0.02d	0.60±0.01b	1.98±0.02c	2.22±0.02c	98.48±0.81c	0.23±0.00c	2.08±0.02a	0.06±0.00c	4.25±0.04a	122.23±1.07c
7-6	0.25±0.06e	6.42±0.05b	1.97±0.01c	1.24±0.01c	14.03±0.10b	10.48±0.07b	0.88±0.01b	5.60±0.04b	3.21±0.02b	95.46±4.66b	3.58±0.03b	0.41±0.00d	0.70±0.005b	1.23±0.01b	144.22±5.02b
7-7	0.84±0.03b	13.04±0.06a	4.40±0.02a	3.04±0.01a	14.45±0.17a	13.70±0.06a	3.10±0.01a	8.65±0.04a	4.79±0.02a	125.41±2.58a	14.97±0.07a	0.207±0.00e	10.59±0.05a	0.11±0.001d	217.17±3.02a
SC															
7-1	0.93±0.05d	0.09±0.02g	—	0.15±0.03g	0.25±0.14g	0.63±0.35f	0.33±0.08e	0.14±0.07c	0.07±0.04g	—	—	0.20±0.12e	0.01±0.00e	0.01±0.00b	2.81±0.13g
7-2	1.12±0.10c	0.48±0.04e	0.04±0.00e	0.28±0.03f	2.76±0.24f	3.92±0.34d	1.23±0.11c	0.57±0.03d	0.34±0.03f	—	—	1.34±0.12b	—	—	11.50±0.07f
7-3	0.86±0.06d	0.63±0.05d	—	0.42±0.03e	2.08±0.16e	2.53±0.19e	3.28±0.25a	—	1.88±0.14e	0.28±0.02e	—	1.39±0.10b	0.04±0.00d	0.05±0.00a	13.37±0.33e
7-4	0.97±0.03d	0.24±0.01f	0.50±0.01d	1.01±0.03b	4.35±0.16d	2.53±0.07e	0.41±0.01e	1.06±0.03b	4.310±0.11b	20.51±0.54d	—	1.78±0.05a	0.04±0.00d	0.05±0.00a	37.70±0.28d
7-5	0.99±0.01d	1.78±0.02b	1.08±0.01c	0.62±0.01d	9.28±0.10c	5.35±0.06c	0.73±0.01d	—	2.20±0.03d	65.87±0.74c	—	0.78±0.01d	0.59±0.01b	—	89.28±0.25c
7-6	1.96±0.02a	1.52±0.01c	1.54±0.01b	0.78±0.01c	13.18±0.10b	10.54±0.08b	0.72±0.01d	1.20±0.01a	3.81±0.03c	93.75±1.70b	5.17±0.04b	—	0.49±0.00c	—	134.64±0.36b
7-7	1.60±0.01b	7.07±0.07a	4.30±0.02a	2.87±0.01a	17.85±0.07a	21.00±0.09a	1.89±0.01b	—	11.05±0.05a	143.44±1.60a	20.80±0.09a	0.90±0.004c	8.30±0.03a	—	241.03±2.07a
QH															
7-1	1.00±0.19b	0.35±0.03d	—	0.78±0.07e	3.38±0.32d	3.47±0.33b	0.69±0.07a	—	—	—	—	0.94±0.09d	—	—	10.61±0.72f
7-2	0.90±0.01b	0.25±0.03e	—	1.14±0.12d	3.16±0.34d	2.75±0.29d	0.44±0.05c	—	—	—	—	0.66±0.07e	0.12±0.01b	—	9.41±0.64f

7-3	0.90±0.05b	0.26±0.02e	0.03±0.00d	0.54±0.03f	5.15±0.31c	3.26±0.20c	0.58±0.03b	—	—	4.76±0.29e	—	1.22±0.07c	—	—	16.69±0.14e
7-4	—	—	0.71±0.11c	0.75±0.01e	2.72±0.03e	1.65±0.02g	0.43±0.02c	3.51±0.04d	—	70.09±0.86d	—	1.29±0.02c	—	—	81.11±0.34d
7-5	0.76±0.01c	0.67±0.01c	1.29±0.11b	2.54±0.02c	3.66±0.03d	1.81±0.01f	—	12.31±0.10c	—	105.70±0.82c	0.06±0.00c	0.58±0.01f	—	—	129.38±1.11c
7-6	0.62±0.00d	5.63±0.02b	0.87±0.00c	4.48±0.01b	8.62±0.03b	2.21±0.01e	0.18±0.001d	37.79±0.81b	0.76±0.002b	262.21±1.80b	6.23±0.02b	2.39±0.01b	—	—	331.99±3.29b
7-7	1.71±0.00a	42.95±0.04a	2.69±0.10a	8.04±0.01a	23.88±0.02a	10.39±0.01a	—	86.19±0.48a	4.86±0.01a	751.22±3.07a	39.86±0.04a	2.29±0.10a	51.55±0.05a	—	1025.62±3.71a
GS															
7-1	2.43±0.17a	0.60±0.04c	0.34±0.02e	—	4.17±0.29c	2.86±0.13e	0.57±0.20d	—	0.24±0.02e	—	—	2.21±0.12c	0.23±0.02d	1.04±0.07b	13.66±0.21g
7-2	1.28±0.04b	3.17±0.10b	0.71±0.02b	0.96±0.03a	4.20±0.45c	5.88±0.19b	0.27±0.10e	—	1.00±0.03d	—	—	3.47±0.02b	0.26±0.11d	1.40±0.05a	21.36±0.19f
7-3	2.23±0.16a	0.61±0.02c	0.44±0.01d	0.22±0.01d	3.26±0.34d	3.75±0.09c	1.22±0.12c	—	0.45±0.01f	10.60±0.27e	—	6.06±0.07a	0.44±0.11c	1.41±0.04a	29.35±0.11e
7-4	1.20±0.04b	0.28±0.01d	0.55±0.02c	0.70±0.02b	4.89±0.14b	1.94±0.06f	—	—	1.33±0.04c	21.45±0.62d	—	2.12±0.06c	—	0.07±0.01d	34.45±0.64d
7-5	0.10±0.00e	—	0.20±0.07e	0.34±0.01c	3.00±0.05d	3.12±0.05d	0.09±0.03f	—	2.52±0.04b	46.86±1.94c	0.18±0.00c	1.46±0.02d	0.32±0.06cd	—	58.19±1.02c
7-6	0.40±0.00c	3.35±0.26b	0.19±0.09e	0.97±0.01a	5.82±0.05a	11.76±0.09a	2.43±0.02b	9.61±0.07a	2.57±0.02b	88.23±0.68b	4.12±0.03b	—	1.22±0.01b	0.08±0.001d	130.65±0.53b
7-7	0.29±0.00d	9.13±0.04a	0.93±0.004a	0.35±0.02c	4.03±0.02c	16.34±0.00g	5.75±0.02a	9.30±0.04b	4.46±0.02a	112.36±1.53a	7.44±0.04a	—	61.45±0.29a	0.15±0.001c	231.95±2.14a
DL															
7-1	1.06±0.08a	0.93±0.07d	0.18±0.013c	0.37±0.03e	6.25±0.46b	2.01±0.15d	0.98±0.07b	—	—	—	—	1.00±0.09b	0.56±0.04b	0.25±0.02a	13.32±0.14e
7-2	0.74±0.17b	0.36±0.03e	0.06±0.01e	0.44±0.04d	5.92±0.53bc	1.77±0.16e	1.01±0.09b	—	—	—	—	0.74±0.07c	0.12±0.01c	—	11.27±0.11f
7-3	0.18±0.03e	0.23±0.07e	0.14±0.02d	0.47±0.08d	2.21±0.38e	0.96±0.16g	0.29±0.05d	—	0.04±0.01e	0.71±0.11e	—	0.64±0.11c	0.11±0.02c	0.05±0.01b	6.02±0.20g
7-4	0.15±0.02e	0.17±0.03f	0.10±0.03d	0.42±0.06d	1.34±0.20f	1.14±0.17f	0.28±0.04d	1.67±0.25d	0.09±0.01d	13.12±0.32d	0.03±0.00d	0.43±0.06d	0.16±0.04c	—	19.09±0.19d
7-5	0.52±0.01d	1.20±0.03c	0.45±0.01a	1.61±0.04b	5.26±0.13c	5.60±0.14c	0.19±0.01e	9.61±0.23c	2.03±0.06c	57.97±3.03c	0.36±0.01c	0.87±0.12c	—	—	85.93±3.60c
7-6	0.36±0.00c	3.19±0.04b	0.05±0.00e	0.77±0.01c	4.52±0.05d	7.53±0.08b	0.46±0.01c	10.19±0.11b	3.34±0.04b	77.35±1.15b	2.83±0.03b	1.14±0.01b	—	—	111.73±1.97b
7-7	0.80±0.01b	9.01±0.05a	0.31±0.00b	2.08±0.01a	16.94±0.10a	17.85±0.10a	1.82±0.01a	22.62±0.23a	6.64±0.04a	172.41±1.95a	11.91±0.07a	1.74±0.01a	2.06±0.01a	—	266.18±2.51a

Note: "—", not detected; values with different letters in the same column of the same variety oil are significantly different ($p < 0.05$).