

Tab. S1: Glucosinolate classes and hydrolysis product types in species of the Brassicales. The plant organs indicated were analyzed for glucosinolates by HPLC after derivatization to desulfoglucosinolates. For the analysis of glucosinolate hydrolysis products, fresh plant material was homogenized in aqueous solution, and dichloromethane extracts of the homogenates were analyzed by GC-MS. Glucosinolates were assigned to structural classes according to the structure of their side chains as follows: **A1**, aliphatic: methylthio-/methylsulfinyl-; **A2**, aliphatic: terminal double bond; **A3**, aliphatic: terminal double bond and 2-hydroxy-group; **A4**, aliphatic: other than A1-A3; **B1**, benzyl-; **B2**, 4-hydroxybenzyl-; **B3**, 2-hydroxy-2-phenylethyl-; **B4**, Phe- and Tyr-derived other than B1-B3; **C**, indolic. Glucosinolate hydrolysis product types are abbreviated as follows: **I**, isothiocyanate; **N**, simple nitrile; **EN**, epithionitrile; **OX**, oxazolidine-2-thione; **T**, organic thiocyanate. An X indicates the identification of at least one representative of a glucosinolate class or a hydrolysis product type in the given plant material (n.i., not investigated). Most species were of the Brassicaceae. For species of other families, the family is given below the species name.

Species	Organ	Structural classes of glucosinolates									Types of glucosinolate hydrolysis products				
		A1	A2	A3	A4	B1	B2	B3	B4	C	I	N	EN	OX	T
<i>Alliaria petiolata</i>	seedlings		X			X				X	X	X	X		X
<i>Alyssum alpestre</i>	leaves roots seeds	X								X X X	X X X				
<i>Arabis glabra</i>	leaves roots seeds	X X X								X X	X				
<i>Barbarea intermedia</i>	leaves roots seeds					X		X X X	X X X	n.i. X	n.i.	n.i.	X n.i. X	n.i.	
<i>Barbarea stricta</i>	leaves roots seeds						X X	X X	X X	X X			X X X		
<i>Barbarea vulgaris</i>	seeds							X	X	X	X			X	
<i>Camelina microcarpa</i>	roots flowers siliques seeds	X X X X								X					
<i>Capsella bursa-pastoris</i>	roots flowers seeds	X		X							X				

Tab. S1, continued

Species	Organ	A1	A2	A3	A4	B1	B2	B3	B4	C	I	N	EN	OX	T
<i>Capsella rubella</i>	leaves seedlings flowers seeds	X X X								X n.i.	n.i.	n.i.	n.i.	n.i.	
<i>Cardamine hirsuta</i>	leaves roots seeds siliques	X X X X	X X X X		X X X X	X X X X		X X X X	X X X X	X X X X	X X X X				
<i>Cardamine impatiens</i>	leaves seeds		X X	X X		X				X	X	X	X		
<i>Cleome hassleriana</i> (Cleomaceae)	leaves roots seeds			X X X	X X X					X X X	X X X				
<i>Cleome spinosa</i> (Cleomaceae)	leaves seeds flowers		X		X X X					X X X	n.i. X	n.i.	n.i.	n.i.	n.i.
<i>Diplotaxis muralis</i>	leaves seeds flowers roots	X X X X	X X X		X X	X				X X X X	X X X X				
<i>Draba aurea</i>	leaves roots seeds	X X n.i.	X X n.i.		n.i.	n.i.	n.i.	n.i.	X X n.i.	X X n.i.			X		
<i>Draba lanceolata</i>	leaves roots seeds	X X n.i.	X X n.i.	X X n.i.		n.i.	n.i.	n.i.	n.i.	X X n.i.	X X n.i.	X	X	X	
<i>Draba muralis</i>	leaves roots seeds						X X		X X X	X X X	X X				
<i>Eruca sativa</i>	leaves seedlings seeds flowers siliques flower buds roots	X X X X X X n.i.	X X X X X X n.i.	X X X X X X n.i.					X n.i. X n.i. n.i. n.i. n.i.	X n.i. X n.i. n.i. n.i. X	n.i.	n.i.	n.i.	n.i.	

Tab. S1, continued

Species	Organ	A1	A2	A3	A4	B1	B2	B3	B4	C	I	N	EN	OX	T
<i>Erysimum cheiri</i>	leaves	X								X	X				
	seeds	X			X					X	X				
	roots	X								X	X				
<i>Erysimum hieraciifolium</i>	leaves	X	X			X				X	X				
	seeds	X	X							X	X				
	roots	X	X							X	X	X			
<i>Iberis amara</i>	leaves	X								X	X				
	seeds	X								X	X				
	flowers	n.i.	X	X											
	roots	X								X	X	X			
<i>Isatis tinctoria</i>	leaves	n.i.	X	n.i.	X	n.i.	n.i.								
	seedlings		X	X	X					X	n.i.		n.i.	n.i.	n.i.
	seeds		X	X	X					X	n.i.		n.i.	n.i.	n.i.
	roots	n.i.	X												
<i>Limnanthes douglasii</i> (Limnanthaceae)	leaves									X	X	X			
	seeds									X	X	X			
	roots									X	X	X			
<i>Moringa oleifera</i> (Moringaceae)	leaves		X			X	X			X	n.i.	n.i.	n.i.	n.i.	n.i.
	seeds						X								
<i>Reseda lutea</i> (Resedaceae)	leaves					X				X					
	seeds					X	X			X					
	roots					X	X			X					
<i>Reseda luteola</i> (Resedaceae)	leaves									X			X		
	seeds	n.i.	n.i.	n.i.	n.i.	n.i.	n.i.	X	n.i.	X	n.i.	n.i.	X	X	
	roots							X	n.i.	X	n.i.	X	X	X	
<i>Schouwia purpurea</i>	leaves	n.i.	X	X	X										
	seedlings		X	X	X					X	n.i.	X	X		
<i>Tropaeolum minus</i> (Tropaeolaceae)	leaves	n.i.	X	n.i.	X	n.i.	n.i.								
	seeds					X	X			X	n.i.	X	n.i.	n.i.	n.i.
	flowers					X	X			X	n.i.	X	n.i.	n.i.	n.i.