

Supplemental material

Fig. S1. Further glucosinolates

Those coded structures in brackets with numbering <200 are already known and have been covered earlier, those with number codes >200 are extrapolations, to complete each new homologous series.

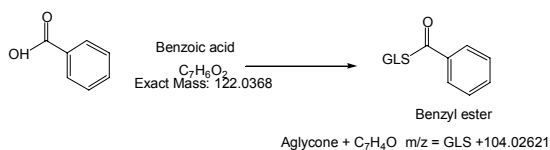
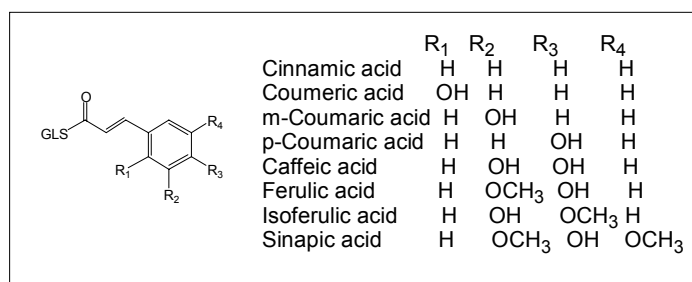
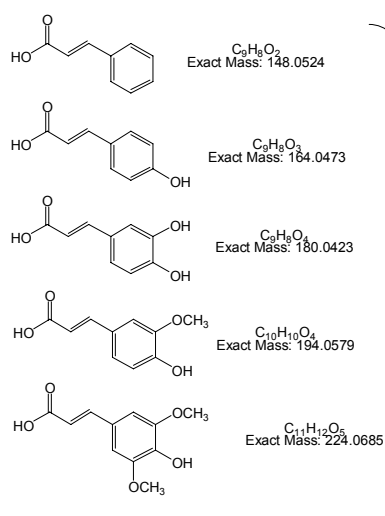
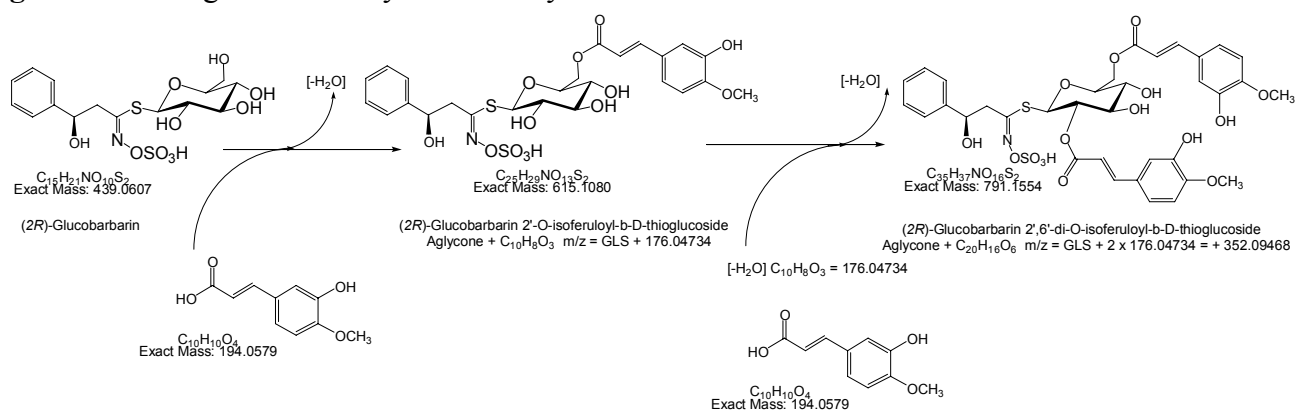
A. Sulfur containing side-chains

	Methyl-thio-alkene	Methyl-thio-hydroxy-alkyl	Methyl-thio-oxo-alkyl	Methyl-sulfinyl-alkene	Methyl-sulfinyl-hydroxy-alkyl	Methyl-sulfinyl-oxo-alkyl	Methyl-sulfonyl-alkene	Methyl-sulfonyl-hydroxy-alkyl
n								
1	201	210	218	225	234	242	250	259
2	[83]	211	219	[63]	235	243	[75]	[260*]
3	202	212	220	226	236	244	251	261
4	203	[37]	221	227	[33]	245	252	[35]
5	204	[36]	[91]	228	[32]	246	253	[34]
6	205	213	[90]	229	237	[70]	254	262
7	206	214	[93]	230	238	[71]	255	263
8	207	215	222	231	239	247	256	264
9	208	216	223	232	240	248	257	265
10	209	217	224	233	241	249	258	266

	Methyl-sulfonyl-oxo-alkyl	Butenyl-thio-alkene	Benzyl-sulfonyl-alkene	Glucosyl-disulfanyl-alkyl	Dimer mercapto	Cysteinyl-thio-alkyl	Glycyl-thio-alkyl
n							
1	267	277	286	295	304	313	322
2	268	278	287	296	305	314	[323*]
3	269	279	[181]	297	306	315	324
4	270	280	288	[135]	[136]	[121]	325
5	271	281	289	298	307	316	326
6	272	282	290	299	308	317	327
7	273	283	291	300	309	318	328
8	274	284	292	301	310	319	329
9	275	[182]	293	302	311	320	330
10	276	285	294	303	312	321	331

	Mercapto-alkyl	Cysteinyl-disulfanyl-alkyl	Glutathione-disulfanyl-alkyl	Methylsulfonyl-hydroxy-alkene	Aspartyl-cysteinyl-disulfanyl-alkyl
n					
1	332	341	350	359	369
2	333	342	351	360	370
3	334	343	352	361	371
4	[185]	[186]	[187]	362	372
5	335	344	353	363	373
6	336	345	354	364	374
7	337	346	355	365	375
8	338	347	356	366	376
9	339	348	357	367	377
10	340	349	358	368	378

Fig. S2. Screening for cinnamoyl and benzoyl esters



Cinnamoyl acid	Formulae Acid	Formulae Ester	Mass gain Mono-ester	Mass gain Di-ester
Cinnamic acid	C ₉ H ₈ O ₂	C ₉ H ₆ O	130.04186	260.08372
Coumaric acid	C ₉ H ₈ O ₃	C ₉ H ₆ O ₂	146.03678	292.07356
Caffeic acid	C ₉ H ₈ O ₄	C ₉ H ₆ O ₃	162.03169	324.06338
Ferulic acid	C ₁₀ H ₁₀ O ₄	C ₁₀ H ₈ O ₃	176.04734	352.09468
Isoferulic acid	C ₁₀ H ₁₀ O ₄	C ₁₀ H ₈ O ₃	176.04734	352.09468
Sinapic acid	C ₁₁ H ₁₂ O ₅	C ₁₁ H ₁₀ O ₄	206.05791	412.11582

<i>Brassica rapa</i> var. <i>ruvo</i>	Rapini (Broccoli raab)			CN seeds
<i>Crambe maritima</i>	Sea kale	Lilly white		CN seeds
<i>Capparis spinosa</i> var. <i>inermis</i>	Capers			Chiltern seeds
<i>Carica papaya</i>	Paw Paw			Chiltern seeds
<i>Carica candamereensis</i>	Mountain paw paw			Chiltern seeds
<i>Cleome spinosa</i>	Spider flower	Sparkler		Jungle seeds
<i>Diplotaxis muralis</i>	Wild Rocket			Thompson & Morgan
<i>Diplotaxis tenuifolia</i>	Wild Rocket			Johnsons seeds
<i>Euruca vesicaria</i> ssp. <i>sativa</i>	Rocket salad	Rocket discovery		Thompson & Morgan
<i>Euruca vesicaria</i> ssp. <i>sativa</i>	Rocket salad	Rocket apollo		Thompson & Morgan
<i>Isatis tinctoria</i>	Woad			CN seeds
<i>Hesperis matronalis</i>	Dame's violet	Sweet rocket		Heritage wild flowers
<i>Lepidium sativum</i>	Cress	Polycress		Thompson & Morgan
<i>Limnanthes douglasii</i>	Poached egg plant			Thompson & Morgan
<i>Moringa oleifera</i>	Horseradish tree			Jungle seeds
<i>Nasturtium officinale</i>	Watercress			Thompson & Morgan
<i>Phytolacca americana</i>	Pokeweed			Chiltern seeds
<i>Phytolacca bogotensis</i>	Pokeberry			Chiltern seeds
<i>Raphanus sativus</i>	Daikon radish	Mooli tsukushi spring cross F1		Thompson & Morgan
<i>Raphanus sativus</i>	Radish	Rudi		Thompson & Morgan
<i>Reseda odorata</i>	Mignonette	Sweet scented		Suttons
<i>Sinapis alba</i>	White mustard	White mustard		Mr Fothergill's
<i>Tropaeolum majus</i>	Nasturtium	Black velvet		Thompson & Morgan
<i>Wasabi japonica</i>	Wasabi (Potted)			Poyntzfield herb nursery

Main UK seed supplier website addresses

enseeds.co.uk	chilternseeds.co.uk	heritagewildflowers.co.uk	johnson-seeds.com
jungleseeds.co.uk	kingsseeds.co.uk	mr-fothergills.co.uk	poyntzfieldherbs.co.uk
suttons.co.uk	taylors-bulbs.com	thompson-morgan.com	