Supporting Information for:

Understanding the phytochemical diversity of plants: Quantification, variation and ecological function

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Table S1. List of studies on phytochemical diversity found in the systematic literature review, including study system, type of phytochemicals measured, analytic method, type of diversity or component thereof measured, and if variation in, or an effect of, diversity was found or not.

General information				Variation		Effects				Ref.
Study system	**Phytochemicals measured**	**Analytic method**	**Measures used**	**Group variation**	**No group variation**	**Positive effect**	**Negative effect**	**No effect**	**Complex effect**	
Artificial diet	Various compounds	-	Richness			Y		Y		1
Lepidium virginicum	Glucosinolates	GC-FID	Richness	Y		Y				2
Nicotiana attenuata	Leaf compounds	LC-MSMS	Shannon	Y						3
Cardamine	Leaf glucosinolates	LC-MS	Richness, evenness, Shannon, Rao's Q, FRic, FDiv	Y		Y	Y	Y		4
Fabaceae, Senecioneae	Various compounds	-	Richness, Shannon	Y						5
Bursera	Leaf VOCs	GC-MS	Shannon, complexity index	Y						6
Zea mays	Root VOCs	GC-MS	Evenness, Simpson	Y					Y	7
Mikania micrantha	Leaf terpene VOCs	GC-MS	Shannon	Y						8
Mikania micrantha	Leaf terpene VOCs	GC-MS	Shannon	Y						9
Streptanthus	Leaf glucosinolates	HPLC	Richness, Shannon, complexity index	Y						10
Artificial diet	Various compounds	-	Richness			Y				11
Piper amalago	Leaf compounds	LC-MS, NMR	Hill-Shannon			Y				12
55 tree species	Leaf VOCs	GC-MS	Richness	Y						13
202 tree species	Leaf terpene VOCs	GC-MS	Richness	Y						14
Annona purpurea	Leaf, stem, root alkaloids	GC-MSMS	Margalef			Y				15
416 plant species	Leaf compounds	LC-MSMS	Richness	Y		Y				16
Gossypium hirsutum	Leaf VOCs	GC-MS	Shannon (joint entropy)						Y	17

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Study system	**Phytochemicals measured**	**Analytic method**	**Measures used**	**Group variation**	**No group variation**	**Positive effect**	**Negative effect**	**No effect**	**Complex effect**	
Erodium cicutarium	Leaf, blossom, fruit terpenes	GC-MS	Shannon	Y						18
Tanacetum vulgare	Floral VOCs, pollen compounds	GC-MS	Richness, Shannon	Y						19
Oenothera cespitosa	Floral VOCs	GC-MS	Richness	Y						20
Nicotiana	Leaf, root, calyx compounds	LC-MSMS	Richness, Shannon	Y						21
Persea americana	Leaf compounds	GC-MS	Evenness, Shannon, Simpson			Y		Y		22
305 plant species	Floral VOCs	-	Richness	Y						23
Juniperus rigida	Needle compounds	GC-MS	Evenness, Shannon, Simpson	Y		Y		Y		24
37 plant species	Leaf compounds	LC-MSMS	Richness			Y	Y	Y		25
Inga	Leaf compounds	LC-MSMS	Functional Hill diversity	Y						26
Quercus ilex	Leaf VOCs, phenolics	HPLC, GC-MS	Shannon	Y				Y		27
Piper kelleyi	Leaf compounds	HPLC	Hill-Shannon	Y					Y	28
Piper kelleyi	Leaf compounds	LC-MS, NMR	Richness, Simpson	Y		Y				29
Solanum Pennellii	Leaf compounds	LC-MS	Simpson			Y				30
Medicago sativa	Leaf compounds	HPLC	Hill-Shannon		Y			Y		31
Medicago sativa	Leaf compounds	LC-MS	Hill-Shannon						Y	32
Pinus sylvestris	Needle terpenes	GC-MS	Shannon, Simpson						Y	33
Apiaceae	Classes of compounds	-	Richness					Y		34
Lupinus polyphyllus	Leaf alkaloids	HPLC	Richness		Y					35
Salix	Leaf compounds	LC-MSMS	Richness	Y		Y				36
Nothofagus	Leaf compounds	TLC	Richness					Y		37

General information				Variation		Effects				Ref.
Study system	**Phytochemicals measured**	**Analytic method**	**Measures used**	**Group variation**	**No group variation**	**Positive effect**	**Negative effect**	**No effect**	**Complex effect**	
Nicotiana attenuata	Compounds (different tissues)	LC-MSMS	Shannon	Y						38
Nicotiana attenuata	Leaf compounds	LC-MSMS	Shannon	Y						39
Phaseolus	Leaf compounds	HPLC	Shannon			Y				40
Phaseolus vulgaris	Leaf compounds	HPLC	Shannon			Y				41
12 Asteraceae species	Leaf compounds	LC-MS	Richness	Y					Y	42
Piper	Leaf compounds	NMR	Simpson						Y	43
Erysimum cheiranthoides	Leaf cardenolides	LC-MS	Evenness	Y						44
Plantago lanceolata	Leaf compounds	LC-MS	Richness, evenness, Shannon, Simpson						Y	45
Brassica nigra	Leaf glucosinolates	HPLC	Shannon	Y					Y	46
Cecropia	Leaf compounds	HPLC	Richness, Shannon	Y						47
Cornus florida	Leaf compounds	LC-MS	Richness, evenness, Shannon, Simpson, Berger-Parker	Y			Y			48
8 trees species	Leaf compounds	LC-MS	Richness, Shannon	Y						49
9 bryophyte species	Moss compounds	LC-MS	Shannon	Y						50
9 bryophyte species	Moss compounds	LC-MSMS	Richness, evenness, Shannon	Y						51
10 bryophyte species	Moss compounds	LC-MSMS	Richness, evenness, Shannon	Y						52
Ceanothus velutinus	Leaf compounds	LC-MS	Hill-Shannon	Y					Y	53
Piper	Leaf compounds	LC-MS, NMR	Hill-Shannon	Y		Y		Y	Y	54
Piper	Leaf compounds	GC-MS	Shannon	Y						55
Apocynum	Root cardenolides	HPLC	Shannon	Y					Y	56

General information				Variation		Effects				Ref.
Study system	**Phytochemicals measured**	**Analytic method**	**Measures used**	**Group variation**	**No group variation**	**Positive effect**	**Negative effect**	**No effect**	**Complex effect**	
Asclepias	Leaf and root cardenolides	HPLC	Shannon	Y						57
Piper	Leaf compounds	NMR	Simpson			Y				58
8 grassland species	Leaf compounds	LC-MS	Richness, Hill-Shannon	Y		Y	Y			59
Medicago sativa	Leaf saponins	LC-MSMS	Richness, Shannon, Simpson	Y						60
Piper	Leaf compounds	GC-MS	Rao's Q (community level)			Y				61
31 Burseraceae species	Leaf compounds	GC-MS, LC-MS	Richness	Y		Y				62
Piper	Leaf compounds	-	Rao's Q (community level)			Y		Y		63
Various plant species	Floral VOCs	-	Richness, Shannon						Y	64
Piper	Leaf and fruit compounds	LC-MSMS	Richness	Y						65
21 tree/shrub species	Leaf phenolics and tannins	HPLC	Shannon					Y		66
Piper	Leaf compounds	NMR	Simpson						Y	67
Asclepias	Leaf cardenolides	HPLC	Shannon						Y	68
Bunias orientalis	Leaf glucosinolates	LC-MS	Shannon			Y				69
Bunias orientalis	Leaf glucosinolates	LC-MS	Shannon	Y	Y					70
Persea americana	Leaf compounds	GC-FID	Shannon					Y		71
Ficus	Leaf compounds	LC-MS(MS)	Shannon	Y					Y	72
Ficus	Leaf compounds	LC-MS(MS)	Shannon	Y					Y	73
Salix	Leaf compounds	LS-MSMS	MPD	Y						74
Glycine max	Plant volatiles	GC-MS	Shannon, Simpson, Brillouin, McIntosh	Y		Y				75
4 tree species	Leaf and root compounds	LC-MS	Richness, Shannon	Y						76

General information				Variation		Effects				Ref.
Study system	**Phytochemicals measured**	**Analytic method**	**Measures used**	**Group variation**	**No group variation**	**Positive effect**	**Negative effect**	**No effect**	**Complex effect**	
Malus	Fruit phenolics	HPLC	Shannon			Y				77
Piper reticulatum	Leaf, root, flower, fruit, seed amides	GC-MS	Richness	Y						78
Artificial diet	Phenolics	-	Richness, evenness, MPD			Y		Y		79
Tanacetum vulgare	Leaf terpenes	GC-MS	Shannon, evenness (of chemotypes)	Y						80
Tanacetum vulgare	Leaf compounds	GC-MS	Shannon	Y	Y					81
Ficus	Fig VOCs	-	Shannon (conditional entropy)						Y	82
Primula Oreodoxa	Floral VOCs	GC-MS	Richness	Y						83
315 tree species	Root compounds	LC-MSMS	Shannon	Y					Y	84
Tanacetum vulgare	Leaf terpenes	GC-MS	Shannon (individual and community level)			Y	Y	Y		85
20 plant species	Leaf VOCs	GC-MS	Shannon (conditional entropy)						Y	86
Erysimum	Leaf glucosinolates, cardenolides	GC-MS	Richness	Y						87

Study system describes the system in which the study was performed. *Phytochemicals measured* describes what kind of tissue samples were taken from, and what kind of compounds were measured (if applicable; this includes biosynthetic class and if compounds were Volatile Organic Compounds (VOCs)). *Analytic method* describes what kind of analytic method compounds were analysed with. *Measures used* describes which diversity indices, or components of diversity, were measured (MPD: mean pairwise dissimilarity, Hill-Shannon: Hill diversity at q = 1, which corresponds to the exponential of Shannon's diversity). *Group variation* indicates that variation was found between groups, e.g. populations, species, treatments and tissues (*Y* indicates Yes). *No group variation* indicates that no variation was found between groups, e.g. populations, species, treatments and tissues, when it was tested for. *Positive effect*, *Negative effect* and *No effect* indicates whether there was direct evidence of positive, negative or no effect, respectively, of an increased phytochemical diversity on some aspect (e.g. herbivore resistance) of plant performance. *Complex effect* indicates that (according to our best judgements) effects were variable, complex or difficult to interpret, with uncertain effects on plant performance, or effects that were difficult to relate to plant performance. *Ref.* indicates the reference for the study. If a study tested for variation, there is a *Y* for *Group variation* and/or *No group variation*. If both these cells are empty, this indicates variation was not tested for/not applicable. If a study tested for an effect, there is a *Y* for *Positive effect*, *Negative effect*, *No effect* and/or C*omplex effect*. If all these four cells are empty, this indicates an effect was not tested for/not applicable.

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