Suppelementary Material

Table S1. Basal area weights for varieties 'Loden' and 'Tora' in species mixtures 'Loden':'Tora' at sites Rostock and Uppsala used for calculating net diversity effects (NDE; equation 3).

Site	Variety	Basal area weights
Rostock	'Loden'	0.427558
Rostock	'Tora'	0.572442
Uppsala	'Loden'	0.302752
Uppsala	'Tora'	0.697248

Table S2. Soil chemical characteristics: results of two-way ANOVAs for soil C:N ratios, nutrient concentrations of C, N, K_{dl}, Mg_{dl} and P_{dl} as well as soil CO_2 respiration for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and *p*-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
C:N	(Intercept)	734.03	1	<0.001
	Site	0.04	1	0.850
	Variety composition	1.80	2	0.406
	Site:variety composition	1.61	2	0.447
C	(Intercept)	246.72	1	<0.001
	Site	13.73	1	<0.001
	Variety composition	8.42	2	0.015
	Site:variety composition	3.70	2	0.157
N	(Intercept)	262.50	1	<0.001
	Site	21.13	1	<0.001
	Variety composition	3.00	2	0.223
	Site:variety composition	2.65	2	0.266
K_{dl}	(Intercept)	35.91	1	<0.001
	Site	20.30	1	<0.001
	Variety composition	0.11	2	0.947
	Site:variety composition	1.40	2	0.498
Mg_{dl}	(Intercept)	113.53	1	<0.001
	Site	13.04	1	<0.001
	Variety composition	0.32	2	0.850
	Site:variety composition	1.49	2	0.474
P_{dl}	(Intercept)	137.34	1	<0.001
	Site	0.03	1	0.858
	Variety composition	0.75	2	0.688
	Site:variety composition	1.16	2	0.561
CO2 respiration	(Intercept)	1.47	1	0.225
	Variety composition	0.15	2	0.926
	Grass cover	0.78	1	0.377

Table S3. Py-FIMS parameters: results of two-way ANOVAs for TII (total ion intensity; 106 counts mg^{-1}) and total thermal stability of bulk SOM (ions volatilized > 400 °C / ions volatilized 50-650 °C), VM (volatile matter), H′ (SOM chemical diversity) and hexoses:pentoses (ratio of microbial- to plant-derived sugars) for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and *p*-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
TII	(Intercept)	111.12	1	<0.001
	Site	41.15	1	<0.001
	Variety composition	8.26	2	0.016
	Site:Variety composition	14.12	2	0.001
Total thermal stability	(Intercept)	180.40	1	<0.001
	Site	5.07	1	0.024
	Variety composition	6.34	2	0.042
	Site:Variety composition	7.39	2	0.025
Chemical diversity	(Intercept)	27926.60	1	<0.001
	Site	14.23	1	<0.001
	Variety composition	4.36	2	0.113
	Site:Variety composition	6.86	2	0.032
Hexoses:pentoses	(Intercept)	549.45	1	<0.001
	Site	33.68	1	<0.001
	Variety composition	1.82	2	0.403
	Site:Variety composition	14.12	2	0.001
Volatile matter	(Intercept)	70.44	1	<0.001
	Site	51.54	1	<0.001
	Variety composition	1.92	2	0.382
	Site:Variety composition	34.44	2	<0.001

Table S4. Soil C accumulation: results of a two-way ANOVA of topsoil (0-10 cm depth) C accumulation rates for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and p-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
C accumulation ($Mg\ C\ ha^{-1}\ year^{-1}$)	(Intercept)	43.50	1	<0.001
	Site	2.70	1	0.100
	Variety composition	19.20	2	<0.001
	Site:Variety composition	9.00	2	0.011

Table S5. Principal component regression: results of two-way ANOVAs for principal components (PC1 and PC2 in Figure 2) derived from the relative ion intensity (% TII) of nine compound classes; CHYDR, PHLM, LDIM, LIPID, ALKYL, NCOMP, PEPTI, SUBER, FATTY in Py-FI mass spectra (for abbreviations, see Table 2) in topsoil (0-10 cm depth) for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and *p*-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
PC1	(Intercept)	114.98	1	<0.001
	Site	81.27	1	<0.001
	Variety composition	16.17	2	<0.001
	Site:Variety composition	5.23	2	0.073
PC2	(Intercept)	0.00	1	0.967
	Site	0.00	1	0.969
	Variety composition	0.09	2	0.958
	Site:Variety composition	1.39	2	0.499

Table S6. SOM chemical composition: results of two-way ANOVAs for the relative ion intensity (% TII) of nine compound classes; CHYDR, PHLM, LDIM, LIPID, ALKYL, NCOMP, PEPTI, SUBER, FATTY in Py-FI mass spectra (for abbreviations, see Table 2) in topsoil (0-10 cm depth) for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and *p*-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
CHYDR	(Intercept)	441.20	1	<0.001
	Site	43.20	1	<0.001
	Variety composition	17.90	2	<0.001
	Site:Variety composition	2.90	2	0.240
PHLM	(Intercept)	770.80	1	<0.001
	Site	66.20	1	<0.001
	Variety composition	15.10	2	0.001
	Site:Variety composition	5.00	2	0.081
LDIM	(Intercept)	113.30	1	<0.001
	Site	8.90	1	0.003
	Variety composition	1.90	2	0.388
	Site:Variety composition	14.50	2	0.001
LIPID	(Intercept)	1261.90	1	<0.001
	Site	28.30	1	<0.001
	Variety composition	2.20	2	0.332
	Site:Variety composition	4.20	2	0.125
ALKYL	(Intercept)	735.80	1	<0.001
	Site	51.60	1	<0.001
	Variety composition	6.30	2	0.043
	Site:Variety composition	3.90	2	0.145
NCOMP	(Intercept)	232.90	1	<0.001
	Site	47.00	1	<0.001
	Variety composition	15.70	2	<0.001
	Site:Variety composition	4.80	2	0.091
PEPTI	(Intercept)	223.30	1	<0.001
	Site	78.50	1	<0.001
	Variety composition	11.40	2	0.003
	Site:Variety composition	67.00	2	<0.001
SUBER	(Intercept)	94.50	1	<0.001
	Site	75.40	1	<0.001
	Variety composition	15.00	2	0.001
	Site:Variety composition	18.50	2	<0.001
FATTY	(Intercept)	48.50	1	<0.001
	Site	24.70	1	<0.001
	Variety composition	14.10	2	0.001
	Site:Variety composition	8.80	2	0.012

Table S7. SOM thermal stability: results of two-way ANOVAs for the thermal stability (ions volatilized > 400 °C / ions volatilized 50-650 °C) of nine compound classes; CHYDR, PHLM, LDIM, LIPID, ALKYL, NCOMP, PEPTI, SUBER, FATTY in Py-FI mass spectra (for abbreviations, see Table 2) in topsoil (0-10 cm depth) for the Salix varieties 'Loden' and 'Tora' grown in monoculture and mixture at sites Rostock and Uppsala. The table lists the Chi-square values (Chisq), degrees of freedom (df), and *p*-values for the fixed effects of Site, Variety composition, and their interaction (Site:Variety composition). Significance of parameters is indicated by $p < 0.05$.

Response variable	Model parameter	Chisq	df	*p*-values
CHYDR	(Intercept)	15.70	1	<0.001
	Site	6.60	1	0.010
	Variety composition	2.10	2	0.346
	Site:Variety composition	14.80	2	0.001
PHLM	(Intercept)	105.10	1	<0.001
	Site	10.30	1	0.001
	Variety composition	6.30	2	0.042
	Site:Variety composition	14.30	2	0.001
LDIM	(Intercept)	1382.30	1	<0.001
	Site	4.70	1	0.030
	Variety composition	6.90	2	0.032
	Site:Variety composition	1.80	2	0.409
LIPID	(Intercept)	234.50	1	<0.001
	Site	17.50	1	<0.001
	Variety composition	9.10	2	0.011
	Site:Variety composition	8.80	2	0.012
ALKYL	(Intercept)	268.30	1	<0.001
	Site	9.20	1	0.002
	Variety composition	8.90	2	0.012
	Site:Variety composition	10.60	2	0.005
NCOMP	(Intercept)	46.80	1	<0.001
	Site	13.20	1	<0.001
	Variety composition	2.50	2	0.292
	Site:Variety composition	13.70	2	0.001
PEPTI	(Intercept)	48.80	1	<0.001
	Site	6.30	1	0.012
	Variety composition	2.70	2	0.260
	Site:Variety composition	14.40	2	0.001
SUBER	(Intercept)	191.20	1	<0.001
	Site	2.60	1	0.109
	Variety composition	13.20	2	0.001
	Site:Variety composition	32.20	2	<0.001
FATTY	(Intercept)	3.20	1	0.073
	Site	1.30	1	0.258
	Variety composition	8.70	2	0.013
	Site:Variety composition	0.30	2	0.841

Table S8. Py-FI marker signals (*m*/*z*) for nine compound classes; CHYDR, PHLM, LDIM, LIPID, ALKYL, NCOMP, PEPTI, SUBER, FATTY (for abbreviations, see Table 2).

Compound class	Py-FI marker signals (*m*/*z*)
CHYDR	60, 61, 72, 82, 84, 96, 98, 110, 112, 114, 126, 132, 144, 162, 163
PHLM	94, 108, 110, 122, 124, 138, 140, 150, 152, 154, 164, 166, 168, 178, 180, 182, 194, 196, 208, 210, 212
LDIM	246, 260, 270, 272, 274, 284, 286, 296, 298, 300, 310, 312, 314, 316, 326, 328, 330, 340, 342, 356
LIPID	202, 216, 230, 244, 256, 258, 270, 272, 284, 286, 298, 300, 312, 314, 326, 328, 340, 342, 354, 368, 380, 382, 394, 396, 408, 410, 422, 424, 438, 452, 466, 480, 494, 508, 522, 536, 550, 564, 578, 592, 606, 620, 634, 648, 662, 676, 704, 718, 732, 746
ALKYL	92, 106, 120, 134, 142, 148, 156, 162, 170, 176, 184, 190, 192, 198, 204, 206, 218, 220, 232, 234, 246, 260, 274, 288, 302, 316, 330, 344, 358, 372, 386
NCOMP	67, 79, 81, 93, 95, 103, 109, 111, 117, 123, 137, 139, 153, 161
PEPTI	58, 59, 70, 73, 74, 75, 84, 87, 91, 97, 115, 120, 129, 135, 167, 185, 203, 243, 276
SUBER	432, 446, 460, 474, 488, 502, 516, 530
FATTY	256, 270, 278, 280, 282, 284, 298, 312, 326, 340, 354, 368, 382, 396, 410, 424, 438, 452, 466, 480, 494, 508

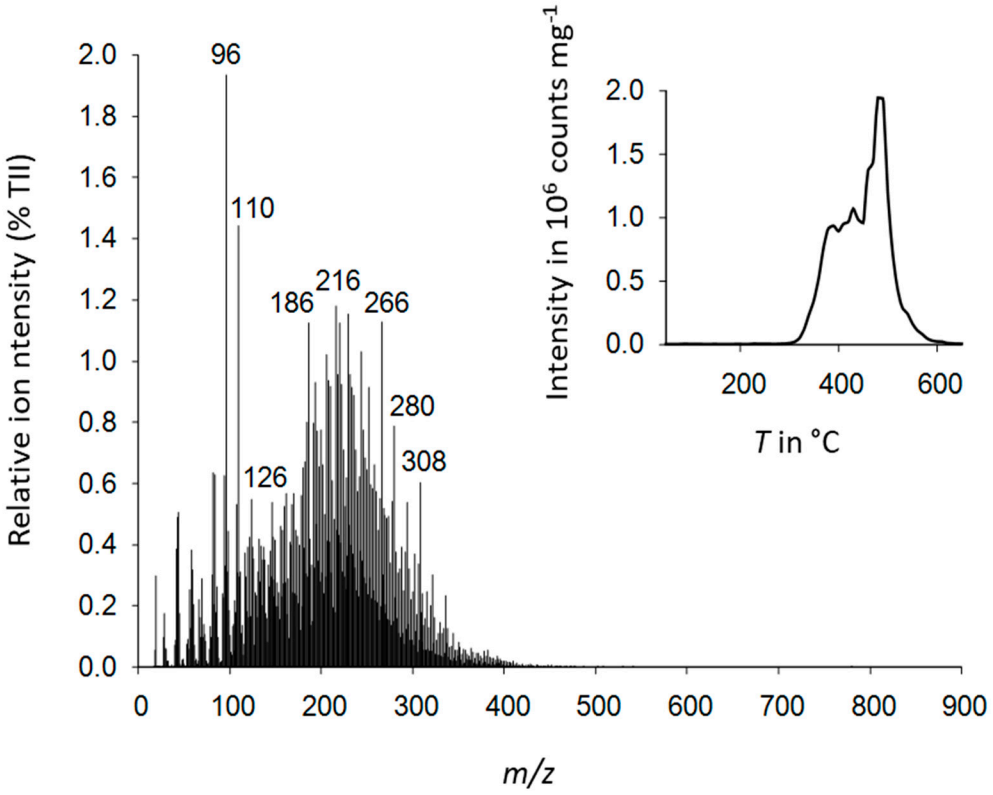


Figure S1. Py-FIMS spectrum with the intensities (% of total ion intensity (TII)) of mass peaks (*m*/*z*) and thermogram (upper right) for soil organic matter from a plot of *Salix* variety 'Tora' at the Uppsala site.

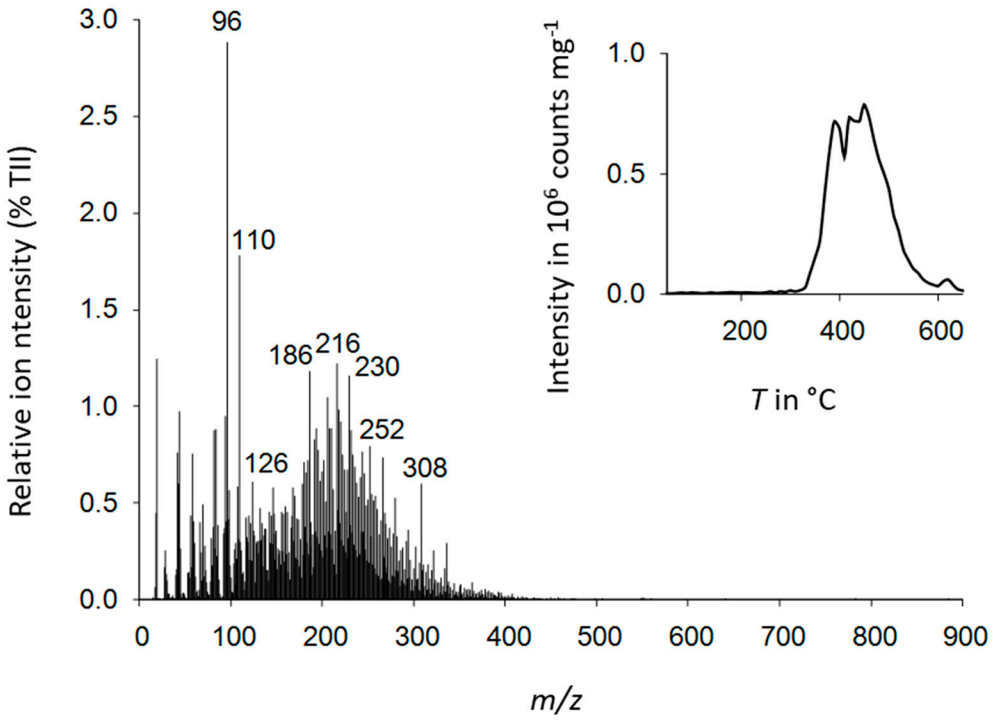


Figure S2. Py-FIMS spectrum with the intensities (% of total ion intensity (TII)) of mass peaks (*m*/*z*) and thermogram (upper right) for soil organic matter from a plot of *Salix* variety mixture 'Loden':'Tora' at the Uppsala site.

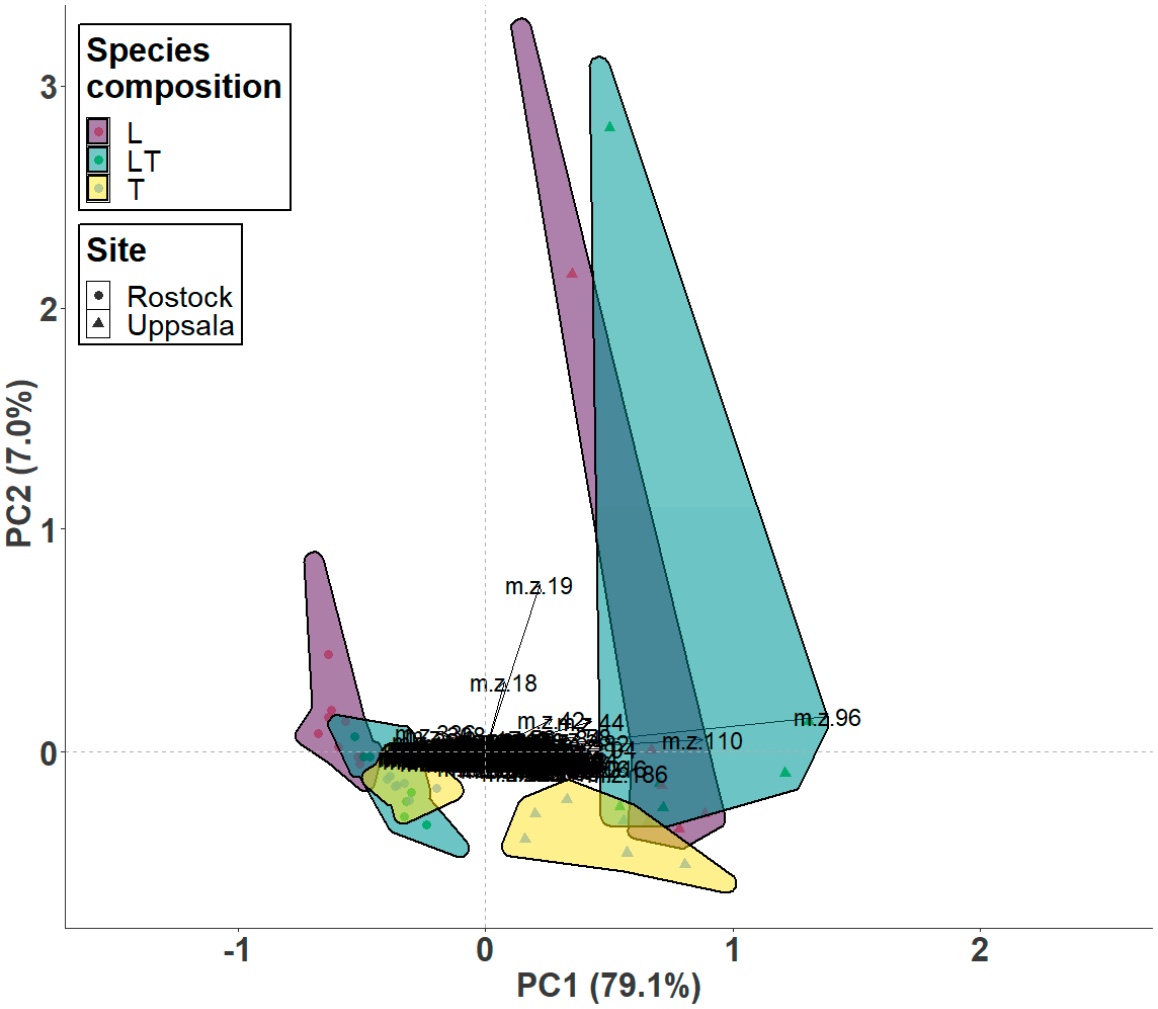


Figure S3. Principal component analysis (PCA) using Py-FI marker signals (*m*/*z*) instead of compound classes.